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Supplemental Information: π-Facial Selectivity in the Diels-Alder Reaction of Glucosamine-based Chiral Furans and Maleimides

Cornelis H. M. van der Loo[a], Rutger Schim van der Loeff[a], Avelino Martín[c], Pilar Gomez-Sal[c], Mark L. G. Borst[b], Kees Pouwer[b] and Adriaan J Minnaard[a,*]

[a] Department of Chemical Biology, Stratingh Institute for Chemistry, University of Groningen, Groningen, The Netherlands. E-mail: A.J.Minnaard@RUG.nl
[b] Symeres B.V., Kadijk 3, 9747 AT Groningen, The Netherlands
[c] Departamento de Química Orgánica y Química Inorgánica, Instituto de Investigación Química "Andres M. Del Rio" (IQAR), Universidad de Alcalá. Alcalá de Henares, 28805, Madrid, Spain

Contents

Material and methods

S1. Reagents

All reagents were acquired from commercial sources and used without further purification. Specifically, D-glucosamine HCl was purchased from Carbosynth Ltd, Silica gel (ultra pure, 40-60 um, 60A), molecular sieves (4 Å), and platinum on activated carbon (5% Pt, not reduced) from Acros Organics, Celite 535 from Carl Roth, phenylboronic acid from AmBeed and *N*-phenylmaleimide from TCI. Thin-layer chromatography (TLC) was carried out on Merck silica gel 60 F254 aluminum plates. Visualization of compounds by TLC was done by potassium permanganate stain. Automated flash column chromatography cartridges were acquired from Screening Devices (UltraPure Irregular Silica Gel, 40 – 63 um, 60A, 5/1P). *N*-benzyloxycarbonyl glucosamine (**GlcNCbz 9**) was prepared according to literature.[1]

*(1) Carbohydr. Res., **1999**, 321, 176–189.*

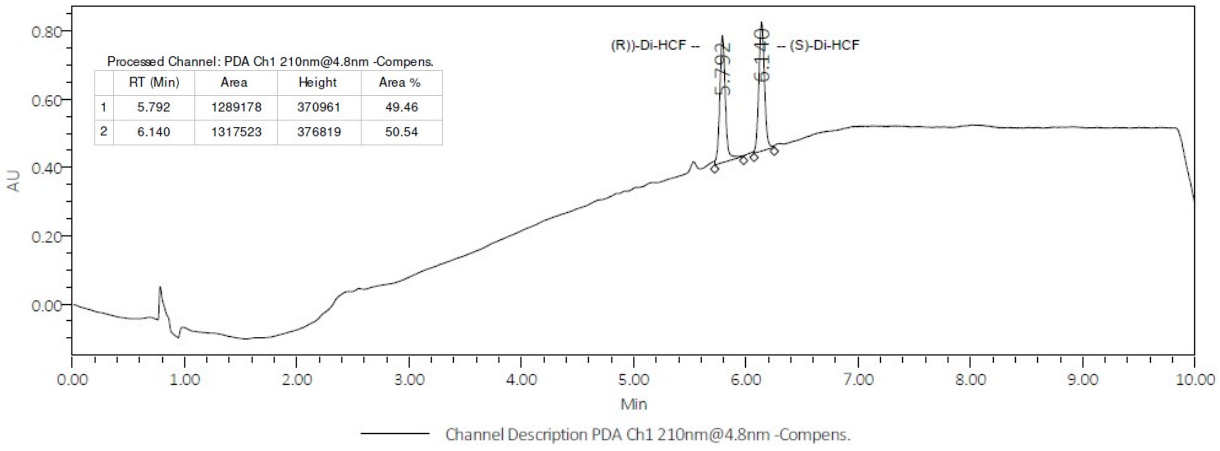
S2. Equipment

^{1}H-NMR and ^{13}C-NMR analyses were performed on a Bruker Avance NEO (400 MHz) at 25 °C. High-resolution mass spectrometry (HRMS) was performed on a Thermo Scientific LTQ Orbitrap XL (FTMS). Infrared spectra (IR) spectra were recorded on a PerkinElmer Spectrum Two FT-IR Spectrometer. DSC was recorded on a TA instruments DSC Q20 and enantiomeric excess (*e.e.*) was determined by chiral HPLC on a waters Acquity UPC^{2}. Automated flash column chromatography was carried out on a Buchi Sepacore® Flash System X10 (Pumps: 601, control unit: 620, detector: 640, fraction collector: 660). Crystal data was collected at 200 K on a Bruker D8 Venture diffractometer equipped with multilayer optics for monochromatization and collimator, Mo Kα radiation (λ = 0.71073 Å) and an Oxford Cryostream 800 unit.

S3. Chiral HPLC method for Di-HCF (**10**)

Chiral SFC Method	:	**31875C UPC² 10m Amy2 EIAN**
System	:	Waters Acquity UPC² system with UV detector and QDA detector
Column	:	Phenomenex Lux Amylose-2 (3.0 x 150 mm; 3 µm)
Mobile Phase A	:	CO_2
Mobile Phase B	:	Ethanol/Isopropanol/Acetonitrile/Ammonium acetate (300 mL/300 mL/300 mL/1.39 g)
Pump Flow	:	1.0 mL/Min
UV detection	:	210 nm
Injection Volume	:	1.0 µL
Total Run Time	:	10.0 Min
Column Temperature	:	40 °C
ABPR	:	138 bar
Mass Detection	:	MS Scan ES positive and negative
Mass Range	:	100 – 600 Da
Pump Program	:	Gradient

Time (Min)	%A	%B	Curve
Initial	98	2	Initial
6.0	60	40	6
9.0	60	40	6
9.1	98	2	6



S4. Crystallographic Data of DAPRED-Bz (**16**)

Crystals of DAPRED-Bz (**16**) were obtained from an ethanol solution (10 mg/mL) as tiny needles. A single crystal was coated with mineral oil, mounted on Mitegen MicroMounts with the aid of a microscope, and immediately placed in the low temperature nitrogen stream of the diffractometer. As crystals diffracted very weakly, data collection was only performed up to theta 25 degrees. Crystallographic data for **16** is presented in table 1.

The structure was solved, by using the Olex2[2] package by intrinsic phasing methods (SHELXT)[3] and refined by least-squares against F^2 (SHELXL).[4] All non-hydrogen atoms were anisotropically refined, while hydrogen atoms that were located in the different Fourier maps were isotropically refined, except those of the phenyl rings which were placed at idealized positions and refined using a riding model.

Table 1. *Experimental data for the X-ray diffraction studies on DAPRED-Bz (**16**).*

	DAPRED-Bz (16)
Formula	C_{31} H_{28} N_2 O_8
M	556.55
T [K]	200(2)
λ[Å]	0.71073
Crystal system	monoclinic
Space group	$P2_1$
a [Å]; α [º]	12.4038(19)
b [Å]; β [º]	6.0006(9); 105.886(4)
c [Å]; γ [º]	18.430(3)
V [Å^3]	1319.3(3)
Z	2
ρ_{calcd} [g cm^{-3}]	1.401
μ [mm^{-1}]	0.102
F(000)	584
Crystal size [mm^3]	0.15 x 0.098 x 0.04
θ range [deg]	3.40 to 25.02
Index ranges	14 to -14, 7 to -7, 21 to -21
Reflections collected	35365
Unique data	4636(R_{int} = 0.145)
Reflections [I>2σ(I)]	3286
Goodness-of-fit on F^2	1.035
Final R indices [I>2σ(I)]	R1 = 0.045 wR2 = 0.080
R indices (all data)	R1 = 0.086 wR2 = 0.096
Largest diff. peak/hole [e·Å^{-3}]	0.164/-0.194

[a] $R1 = \Sigma||F_0|-|F_c||/[\Sigma|F_0|]$ $\quad wR2 = \{[\Sigma w(F_0^2 - F_c^2)^2] / [\Sigma w(F_0^2)^2]\}^{1/2}$

(2) *J. Appl. Cryst.* **2009**, *42*, 339-341.
(3) *Acta Cryst.* **2015**, *A71*, 3-8
(4) *Acta Cryst.* **2015**, *C71*, 3-8

S5. Reversibility Study

In DMSO-d_6 (0.8 mL, 30 mg/mL) solutions were prepared of the *endo* and *exo* diastereomers, as mixtures with matching topologies, of the Diels Alder products of **Di-HCF** (**10**) with *N*-methylmaleimide and *N*-phenylmaleimide. The product distribution was determined at t = 0 by ^{1}H-NMR (table 2). The samples were kept at room temperature, 40 °C, 50 °C, 60 °C and 70 °C. After 24 h, the decrease in concentration of the corresponding isomers was determined by ^{1}H-NMR (table 3). The sum of the concentration of the two target isomers was normalized, and the isomer concentration decrease at each temperature was calculated (table 4, graph 1).

Table 2. *Isomer distribution at t = 0*

Dienophile	Di-HCF	Endo	Endo'	Exo	Exo'	Isomer sum
N-methylmaleimide ***endo***-isomer	0%	**49%**	**49%**	0%	2%	98%
N-methylmaleimide ***exo***-isomer	0%	0%	0%	**26%**	**74%**	100%
N-phenylmaleimide ***endo***-isomer	0%	**45%**	**50%**	0%	5%	95%
N-phenylmaleimide ***exo***-isomer	0%	0%	0%	**23%**	**77%**	100%

Table 3. *Isomer distribution at t = 24h*

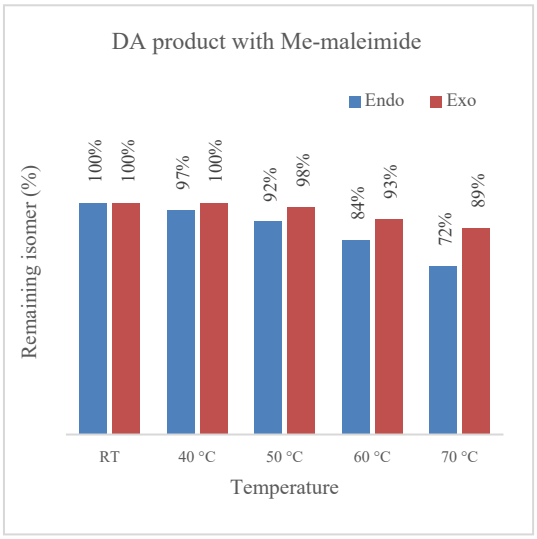
Dienophile	Temperature	Di-HCF	Endo	Endo'	Exo	Exo'	Isomer sum
N-methylmaleimide ***endo***-isomer	RT	0%	**49%**	**49%**	0%	2%	98%
	40 °C	3%	**47%**	**48%**	0%	2%	95%
	50 °C	5%	**44%**	**46%**	2%	3%	90%
	60 °C	7%	**40%**	**42%**	4%	7%	82%
	70 °C	8%	**34%**	**37%**	8%	13%	71%
N-methylmaleimide ***exo*** Endo-isomer	RT	0%	0%	0%	**26%**	**74%**	100%
	40 °C	0%	0%	0%	**26%**	**74%**	100%
	50 °C	2%	0%	0%	**26%**	**72%**	98%
	60 °C	4%	1%	2%	**25%**	**68%**	93%
	70 °C	5%	2%	3%	**24%**	**65%**	89%
N-phenylmaleimide ***endo***-isomer	RT	0%	**45%**	**50%**	0%	5%	95%
	40 °C	6%	**39%**	**45%**	0%	5%	84%
	50 °C	9%	**37%**	**42%**	4%	8%	79%
	60 °C	12%	**29%**	**35%**	8%	16%	64%
	70 °C	14%	**17%**	**21%**	17%	31%	38%
N-phenylmaleimide ***exo***-isomer	RT	0%	0%	0%	**23%**	**77%**	100%
	40 °C	3%	0%	0%	**23%**	**74%**	97%
	50 °C	5%	2%	3%	**22%**	**68%**	90%

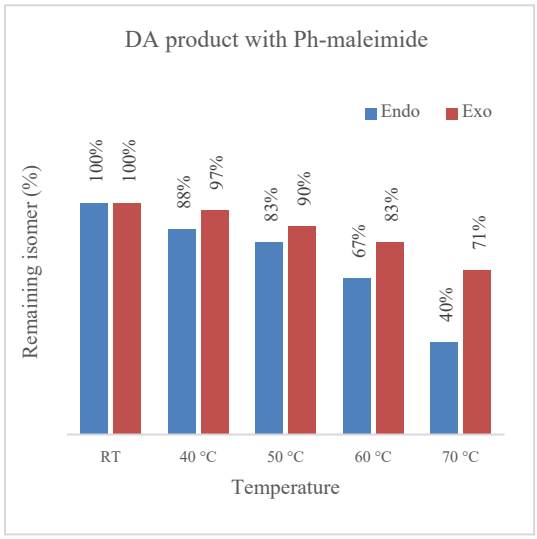
	60 °C	8%	4%	6%	**23%**	**60%**	83%
	70 °C	9%	8%	11%	**24%**	**47%**	71%

Table 4. *Normalized data. Sum of target isomers set to 100% at t=0*

Time & Temperature	*N*-methylmaleimide ***endo***-isomer	*N*-methylmaleimide ***exo***-isomer	*N*-phenylmaleimide ***endo***-isomer	*N*-phenylmaleimide ***exo***-isomer
t = 0	100%	100%	100%	100%
t = 24, RT	100%	100%	100%	100%
t = 24, 40 °C	97%	100%	88%	97%
t = 24, 50 °C	92%	98%	83%	90%
t = 24, 60 °C	84%	93%	67%	83%
t = 24, 70 °C	72%	89%	40%	71%

Graph 1. *Representation of the normalized data from table 4.* ***Left****: The DA product of* ***Di-HCF (10)*** *+ N-methylmaleimide.* ***Right****: The DA product of* ***Di-HCF (10)*** *+ N-phenylmaleimide*





Experimental procedures

S6. Periodate mediated diol oxidation to facilitate NMR analysis

NMR sample preparation. The sample (10 mg substrate) was dissolved in a mixture of DMSO-d_6 – D_2O (1:1. 0.8 mL). To the solution was added $NaIO_4$ (10 mg, ca. 2 eq.) and the mixture was stirred at room temperature for 1 h. The white precipitate was removed by filtration over a disposable syringe filter (0.45 uM) and the filtrate was analyzed by ^{1}H-NMR.

S7. Synthesis of Di-HCF (**10**)

Benzyl (R)-(5-(1,2-dihydroxyethyl)furan-3-yl)carbamate (Di-HCF 10). A mixture was prepared of *N*-benzyloxycarbonyl glucosamine (**GlcNCbz 9**) (95 g, 1 eq., 0.30 mol), phenylboronic acid (55 g, 1.5 eq., 0.45 mol), molsieves (500 g, 4 Å) and pyridine (1 L). Under stirring was added a solution of triflic acid (46 g, 27 mL, 1 eq., 0.30 mol) in pyridine (0.5 L). The mixture was stirred at reflux for 30 min and subsequently cooled to rt. Solid K_2CO_3 (84 g, 2 eq., 0.61 mol) and neopentyl glycol (63 g, 60 mL, 2 eq., 0.61 mol) were added. The suspension was stirred at rt for 1 h. The mixture was filtered over a glass filter (p2) and the filter residue was washed with ethyl acetate until colourless. The filtrate was concentrated to a volume of ca. 500 mL and the brown solution was poured into a suspension of heptanes (2.5 L) and celite (200 g). The solids were filtered off and washed with heptanes (1 L). The filtrate was disposed, and the residue was extracted with ethyl acetate (1.5 L), until colourless. The ethyl acetate filtrate was washed with citric acid (10%, aq., 5 x 500 mL), $NaHCO_3$ (sat., aq., 2 x 500 mL) and brine (500 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo* to afford a brown solid (68 g). The crude product was re-crystallized from DCE (300 mL), the solids were filtered off and the filter cake was washed with small volume of cold DCE. The filter dry solids were dried *in vacuo* (50 °C) to furnish a beige solid (42 g, yield: 50%, purity: 100% (qNMR), 97.4% *ee*). ^{1}H-NMR (400 MHz, DMSO-d6) δ 9.59 (s, 1H), 7.57 (s, 1H), 7.42 – 7.37 (m, 4H), 7.37 – 7.30 (m, 1H), 6.20 (s, 1H), 5.31 (d, 1H), 5.12 (s, 2H), 4.73 (t, 1H), 4.41 (q, 1H), 3.62 – 3.43 (m, 2H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 155.59, 153.72, 137.13, 128.92, 128.68, 128.49, 128.46, 126.24, 101.94, 68.35, 66.38, 64.83. HRMS (ESI) calculated for $C_{14}H_{15}NO_5$ ($M+H^+$):279.1056; found ($M+H^+$): 279.1057.

S8. Synthesis of DAP (**14**)

Benzyl ((3aS,4S,7S,7aR)-7-((R)-1,2-dihydroxyethyl)-1,3-dioxo-2-phenyl-2,3,3a,4,7,7a-hexahydro-1H-4,7-epoxyisoindol-5-yl)carbamate (DAP 14). A solution of N-phenylmaleimide (2.8 g, 1.5 eq., 16 mmol) in chloroform (10 mL) was cooled to -10 °C. To the yellow solution was added benzyl (R)-(5-(1,2-dihydroxyethyl)furan-3-yl)carbamate (**Di-HCF 10**) (3.0 g, 1 eq., 11 mmol) and the resulting suspension was stirred at -10 °C for 16 h. The brown solution was loaded as such on a column cartridge (330 g) and purified by automated flash chromatography (dichloromethane-methanol (0% →6%), figure 1). The combined fractions with product (ca. 0.5 L) were washed with water (4x 300 mL) and brine-water (1:1) (300 mL). The organic phase was dried over Na_2SO_4 and concentrated *in vacuo* (35 °C) to afford the product as an off-white foam (2.8 g, yield: 58%). ^{1}H-NMR (400 MHz, DMSO- d_6) δ 9.92 (s, 1H), 7.53 – 7.45 (m, 2H), 7.45 – 7.38 (m, 5H), 7.38 – 7.31 (m, 1H), 7.24 – 7.19 (m, 2H), 5.93 (s, 1H), 5.21 (s, 1H), 5.13 (s, 2H), 5.12 (d, 1H), 4.53 (t, 1H), 3.98 (dd, 1H), 3.63 – 3.37 (m, 2H), 3.30 (d, 1H), 3.20 (d, 1H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 175.67, 174.31, 153.50, 144.69, 136.70, 132.66, 129.41, 128.96, 128.83, 128.63, 128.57, 127.28, 110.48, 93.87, 80.53, 69.99, 66.77, 63.77, 50.96, 50.24. HRMS (ESI) calculated for $C_{24}H_{22}N_2O_7$ ($M+H^+$): 474.1353; found ($M+H^+$): 474.1344.

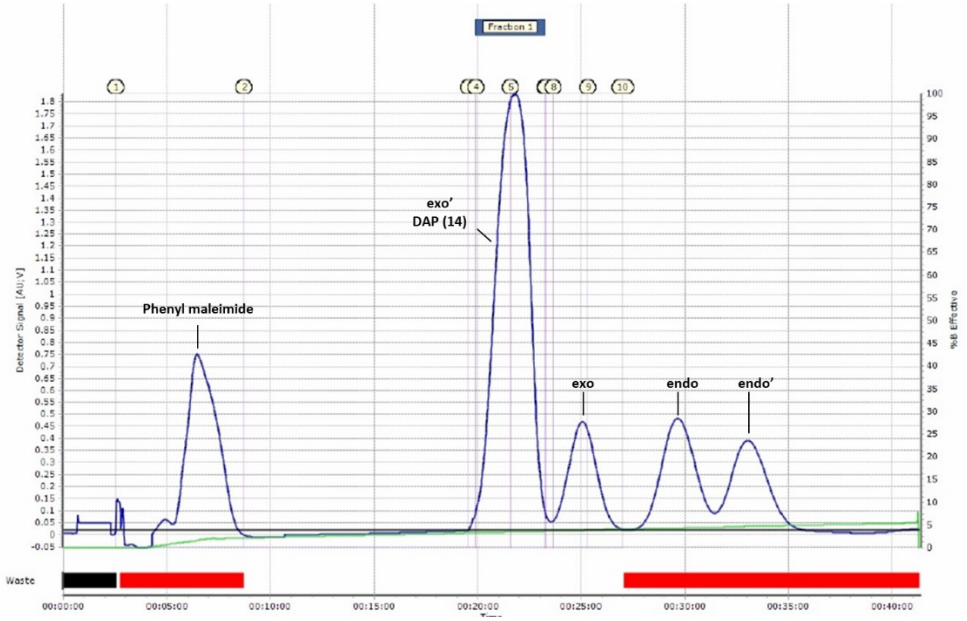


Figure 1. Automated flash chromatography of **DAP** (**14**). Eluent: DCM-MeOH (0% → 6%).

S9. Synthesis of DAPRED (**15**)

Benzyl ((3aS,4S,5S,7S,7aR)-7-((R)-1,2-dihydroxyethyl)-1,3-dioxo-2-phenyloctahydro-1H-4,7-epoxyisoindol-5-yl)carbamate (DAPRED 15). To a solution of benzyl ((3aS,4S,7S,7aR)-7-((R)-1,2-dihydroxyethyl)-1,3-dioxo-2-phenyl-2,3,3a,4,7,7a-hexahydro-1H-4,7-epoxyisoindol-5-yl)carbamate (**DAP 14**) (1.5 g, 1 eq, 3.3 mmol) in THF (20 mL) was added platinum/C (0.32 g, 5% wt., 0.025 eq., 83 µmol). The suspension was placed under a hydrogen atmosphere (1 atm, balloon) and was stirred for 1 h. The mixture was filtered over a disposable syringe filter (0.45 µM) and the filtrate was concentrated *in vacuo* afford a white foam (1.5 g, yield: quant.). ^{1}H-NMR (400 MHz, DMSO- d_6) δ 7.86 (d, 1H), 7.52 – 7.44 (m, 2H), 7.43 – 7.37 (m, 5H), 7.37 – 7.30 (m, 1H), 7.27 – 7.20 (m, 2H), 5.11 (d, 1H), 5.07 (d, 2H), 4.71 (d, 1H), 4.55 (t, 1H), 3.98 (dd, 1H), 3.93 (q, 1H), 3.58 (t, 2H), 3.48 (d, 1H), 3.15 (d, 1H), 2.10 (t, 1H), 1.51 (dd, 1H). ^{13}C-NMR (101 MHz, DMSO- d_6) δ 177.29, 175.57, 156.48, 137.27, 133.00, 129.26, 128.90, 128.70, 128.48, 128.44, 127.28, 91.72, 80.21, 71.86, 66.21, 62.77, 52.13, 50.27, 46.96, 36.94. HRMS (ESI) calculated for $C_{24}H_{24}N_2O_7$ ($M+H^+$): 454.1690; found ($M+H^+$): 454.1690.

S10. Synthesis of DAPRED-Bz (**16**)

(R)-2-((3aR,4S,6S,7S,7aS)-6-(((Benzyloxy)carbonyl)amino)-1,3-dioxo-2-phenyloctahydro-4H-4,7-epoxyisoindol-4-yl)-2-hydroxyethyl benzoate (DAPRED-Bz 16). To a solution of benzyl ((3aS,4S,5S,7S,7aR)-7-((R)-1,2-dihydroxyethyl)-1,3-dioxo-2-phenyloctahydro-1H-4,7-epoxyisoindol-5-yl)carbamate (**DAPRED 15**) (1.5 g, 1 eq.,3.3 mmol) and triethylamine (0.75 g, 1.0 mL, 2.25 eq., 7.5 mmol) in dichloromethane (20 mL) was added benzoyl chloride (0.93 g, 0.77 mL, 2 eq., 6.6 mmol), while maintaining the temperature below 25 °C. The clear mixture was stirred at room temperature for 1 h and subsequently diluted with ethyl acetate (200 mL). The solution was washed with citric acid (10%, aq., 2 x 150 mL), $NaHCO_3$ (sat., aq., 2 x 150 mL) and brine (150 mL). The organic phase was dried over Na_2SO_4 and concentrated *in vacuo* to afford an off-white foam. The crude product was purified by automated column chromatography (40 g column, heptanes-ethyl acetate (0% → 75%)) to afford the product as a white solid (1.5 g, yield: 81%). ^{1}H-NMR (400 MHz, DMSO- d_6) δ 8.04 (d, 2H), 7.91 (d, 1H), 7.70 – 7.61 (m, 1H), 7.53 (t, 2H), 7.51 – 7.49 (m, 1H), 7.49 – 7.45 (m, 2H), 7.44 – 7.30 (m, 5H), 7.25 (d, 2H), 5.77 (d, 1H), 5.09 (s, 2H), 4.78 (d, 1H), 4.46 (td, 2H),

4.41 – 4.32 (m, 1H), 4.10 – 3.94 (m, 1H), 3.53 (d, 1H), 3.27 (d, 1H), 2.25 (t, 1H), 1.60 (dd, 1H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 177.23, 175.31, 166.23, 156.47, 137.23, 133.82, 132.91, 130.17, 129.83, 129.31, 129.16, 128.90, 128.79, 128.51, 128.46, 127.31, 90.95, 80.68, 68.17, 66.30, 66.24, 52.07, 50.49, 46.81, 36.50. HRMS (ESI) calculated for $C_{31}H_{28}N_2O_8$ ($M+H^+$): 558.1952; found ($M+H^+$): 558.1935.

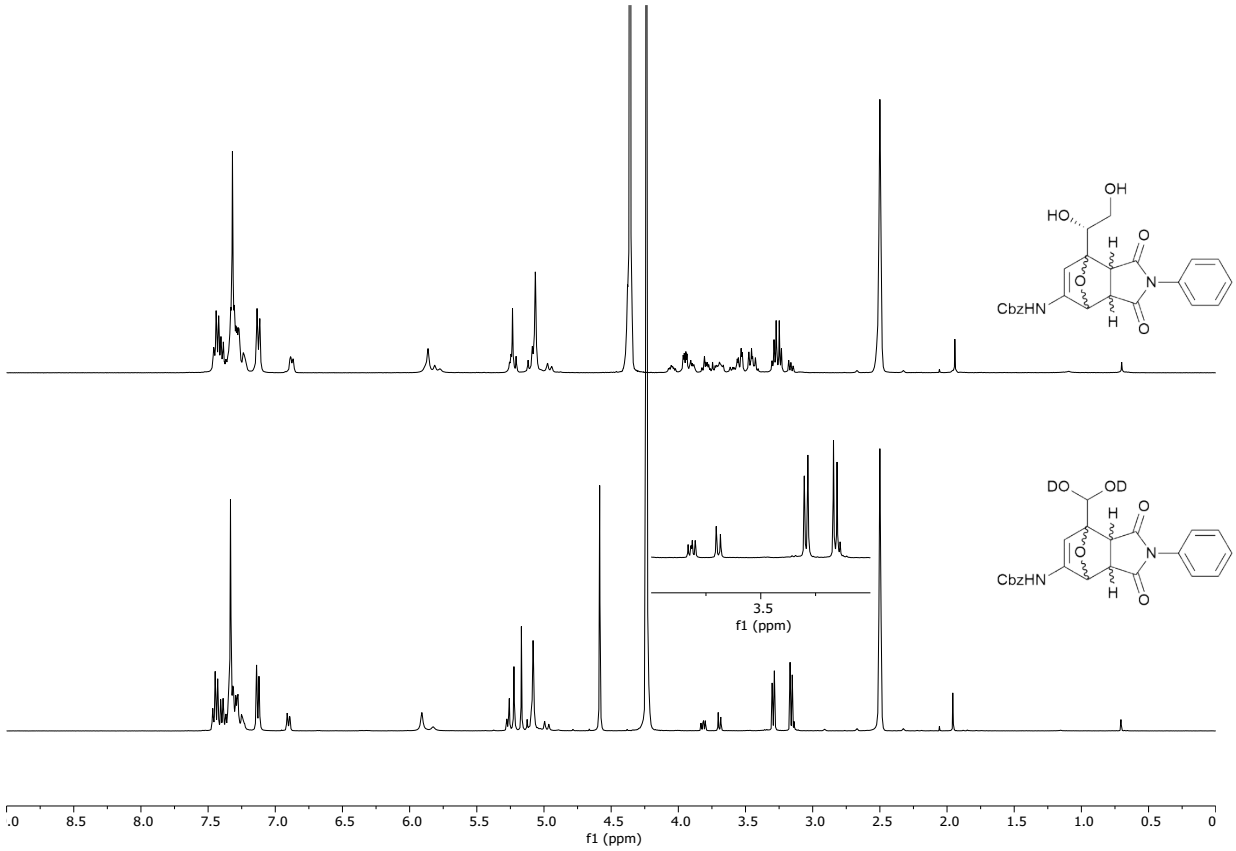
S11. Synthesis of **18**

N-((3aS,4S,7S,7aR)-7-((R)-1,2-dihydroxyethyl)-1,3-dioxo-2-phenyl-2,3,3a,4,7,7a-hexahydro-1H-4,7-epoxyisoindol-5-yl)acetamide (18). A solution of *N*-phenylmaleimide (2.8 g, 1.5 eq., 16 mmol) in chloroform (10 mL) was cooled to -10 °C. To the yellow solution was added dihydroxyethyl acetamidofuran (**Di-HAF** (**1**)) (2.0 g, 1 eq., 11 mmol) and DMSO (1.5 mL). The resulting suspension was stirred at -10 °C for 16 h. The brown solution was poured into a suspension of Celite (6 g) in diisopropyl ether (150 mL). The solids were filtered off and washed with diisopropyl ether (2 x 50 mL) and *tert*-butyl methyl ether (2 x 25 mL). The filter residue was ground to a fine powder with pestle and mortar and was used as solid load for purification by automated flash chromatography (330 g column, dichloromethane-methanol (0% →10%)). The combined fractions with product were extracted with water (3x 200 mL). The aqueous phase was saturated with sodium chloride and subsequently extracted with EtOAc (3 x 300 mL) The organic phase was dried over Na_2SO_4, diluted with toluene (0.5 L) and concentrated *in vacuo* (25 °C) to afford the product as a white solid (2.3 g, yield: 59%). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 10.16 (s, 1H), 7.54 – 7.46 (m, 2H), 7.45 – 7.37 (m, 1H), 7.22 (d, 2H), 6.15 (s, 1H), 5.21 (s, 1H), 5.12 (d, 1H), 4.53 (t, 1H), 4.05 – 3.93 (m, 1H), 3.63 – 3.39 (m, 2H), 3.28 (d, 1H), 3.19 (d, 1H), 1.98 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 175.77, 174.33, 168.86, 144.25, 132.66, 129.41, 128.83, 127.28, 112.28, 93.66, 80.71, 70.01, 63.80, 50.79, 50.26, 23.71. HRMS (ESI) calculated for $C_{18}H_{18}N_2O_6$ ($M+H^+$): 359.1238; found ($M+H^+$): 359.1230.

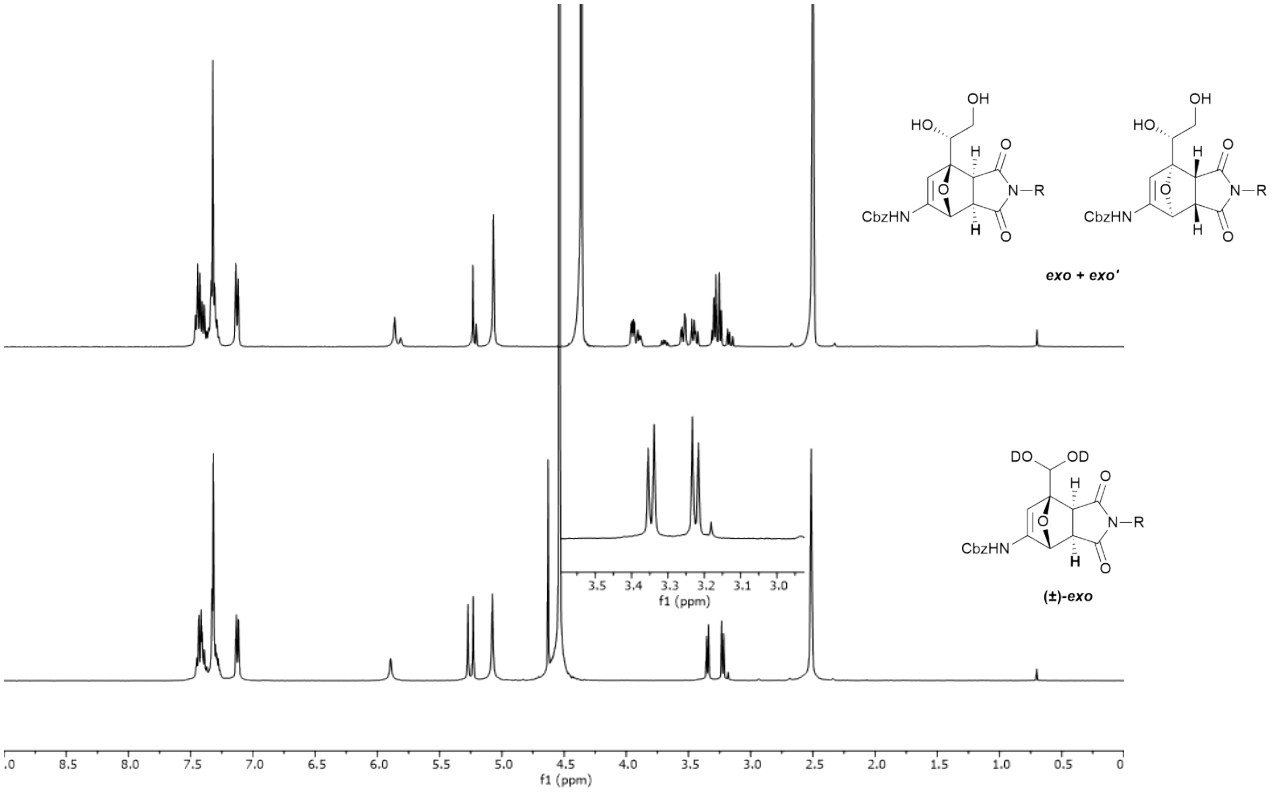
Characterization

S12. Periodate mediated diol oxidation

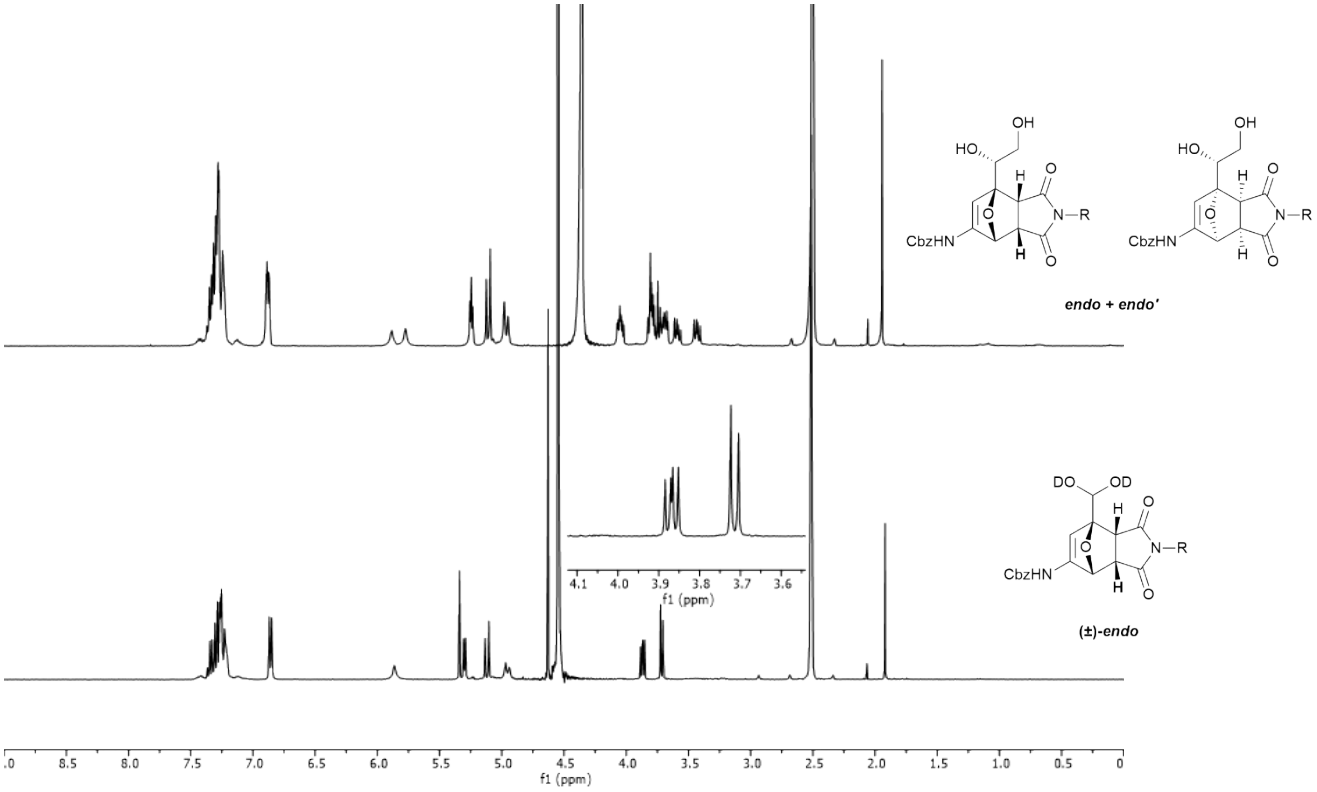
Reaction mixture, *before* & *after*



Exo products, *before* & *after*

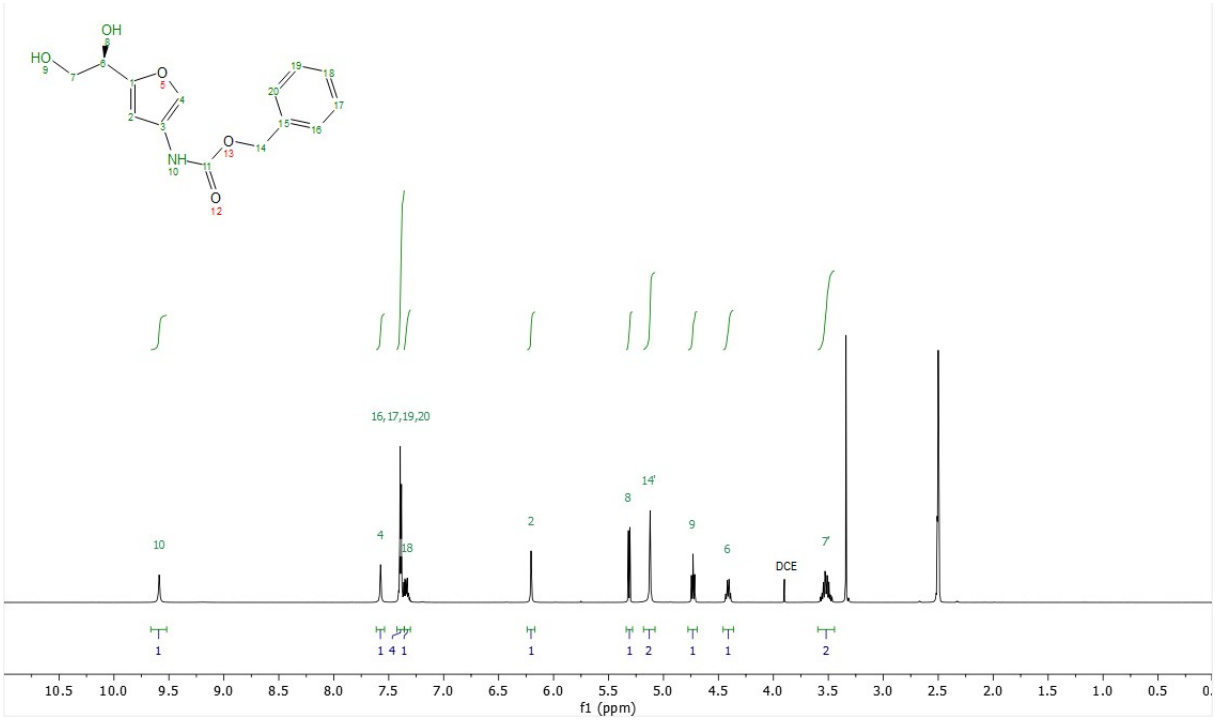


Endo products, *before* & *after*

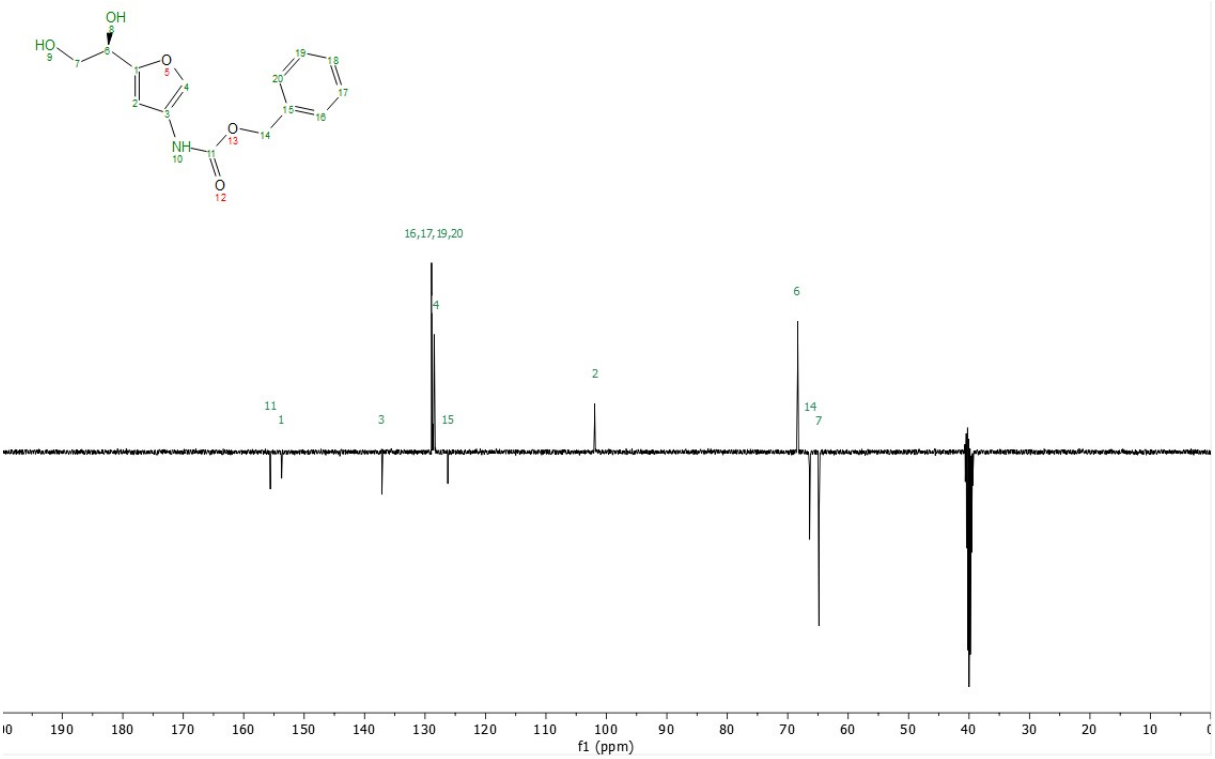


S13. Di-HCF (**10**)

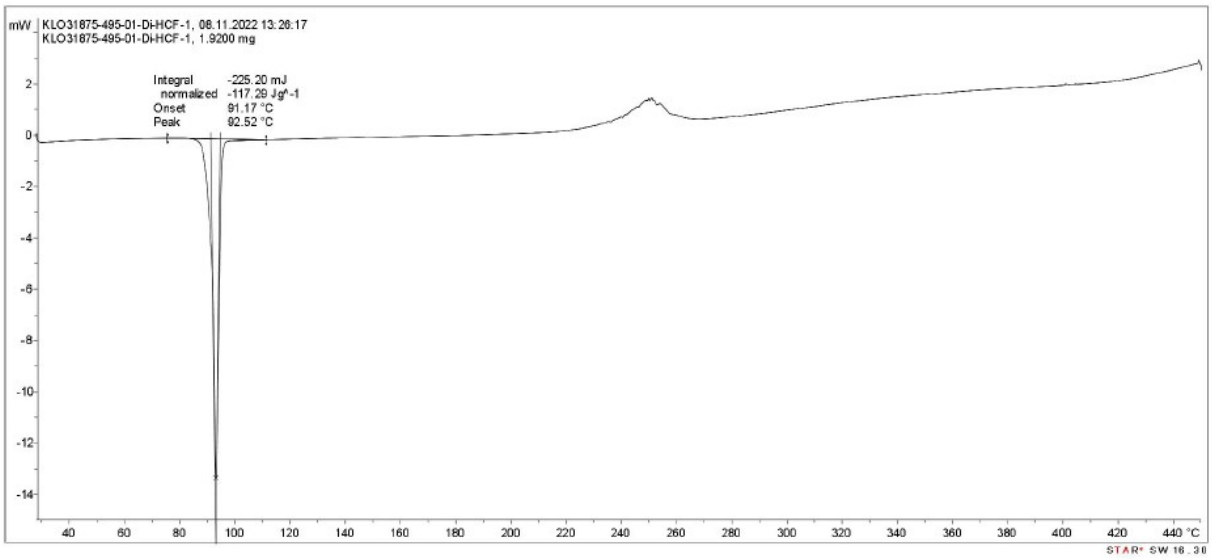
^{1}H-NMR of Di-HCF (**10**) in DMSO-d_6



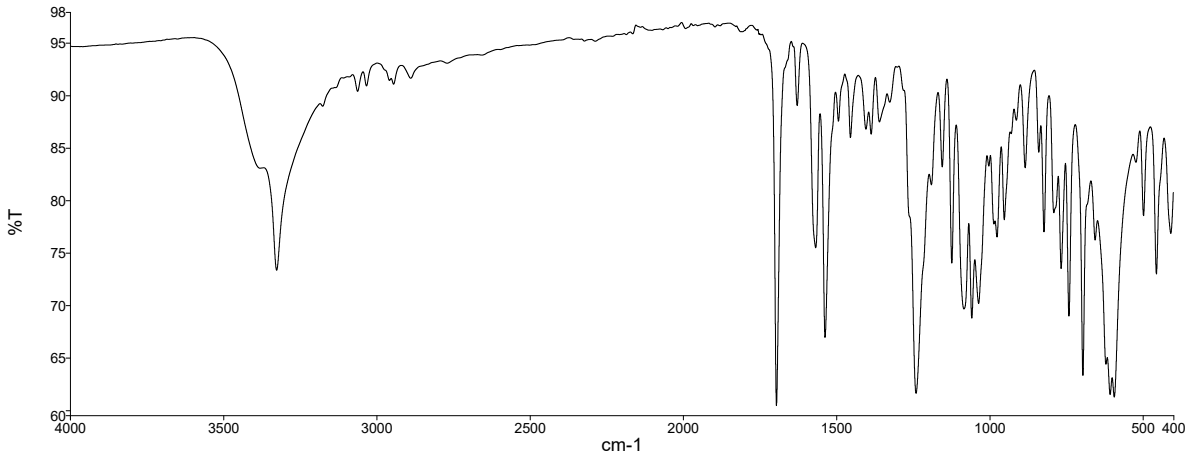
^{13}C-NMR of Di-HCF (**10**) in DMSO-d_6



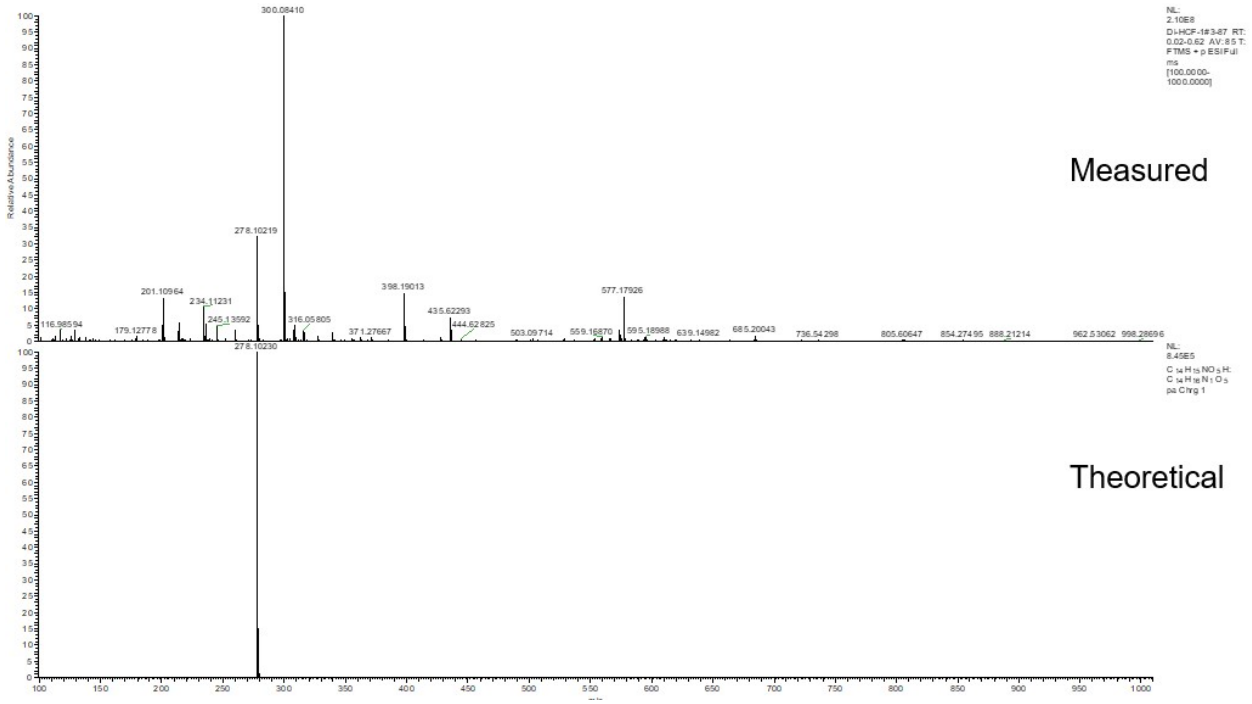
DSC of Di-HCF (**10**)

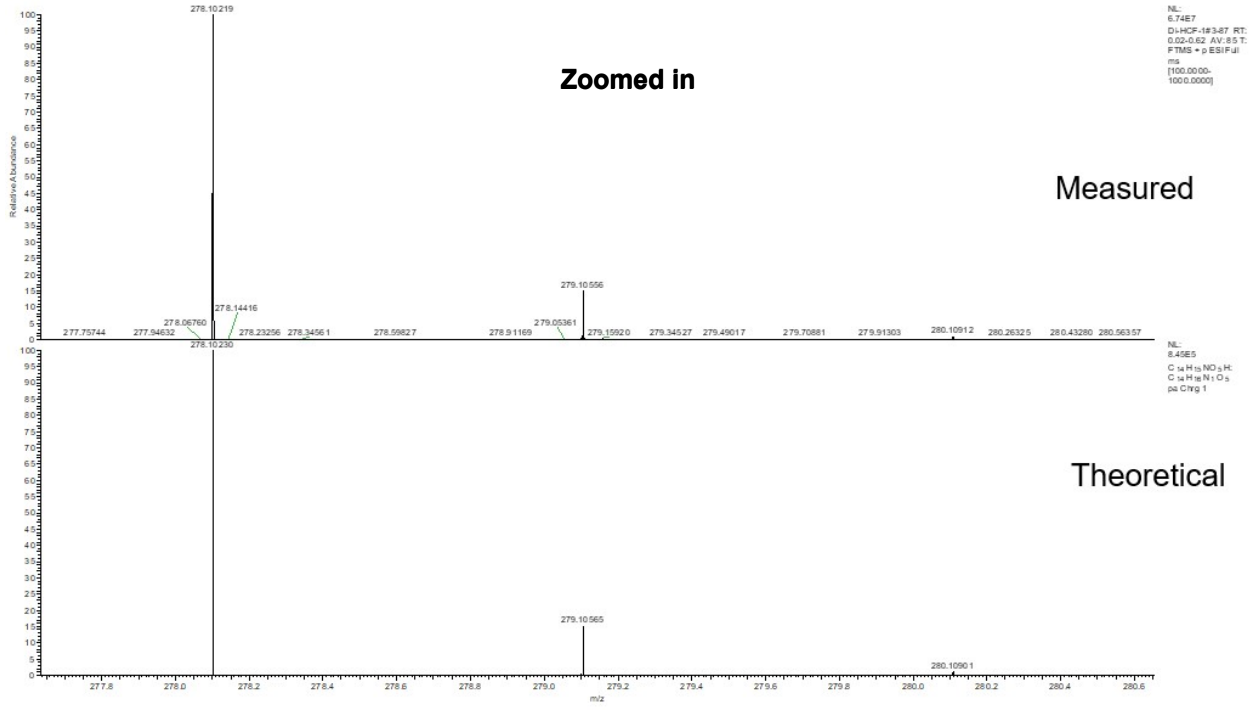


IR of Di-HCF (**10**)

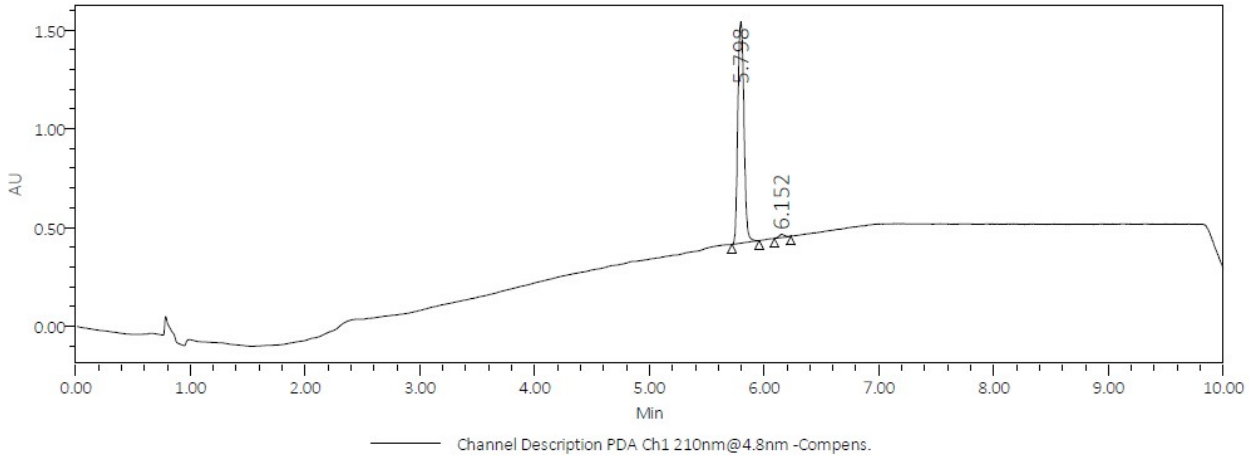


HRMS of Di-HCF (**10**)





Chiral LC analysis of Di-HCF (**10**)

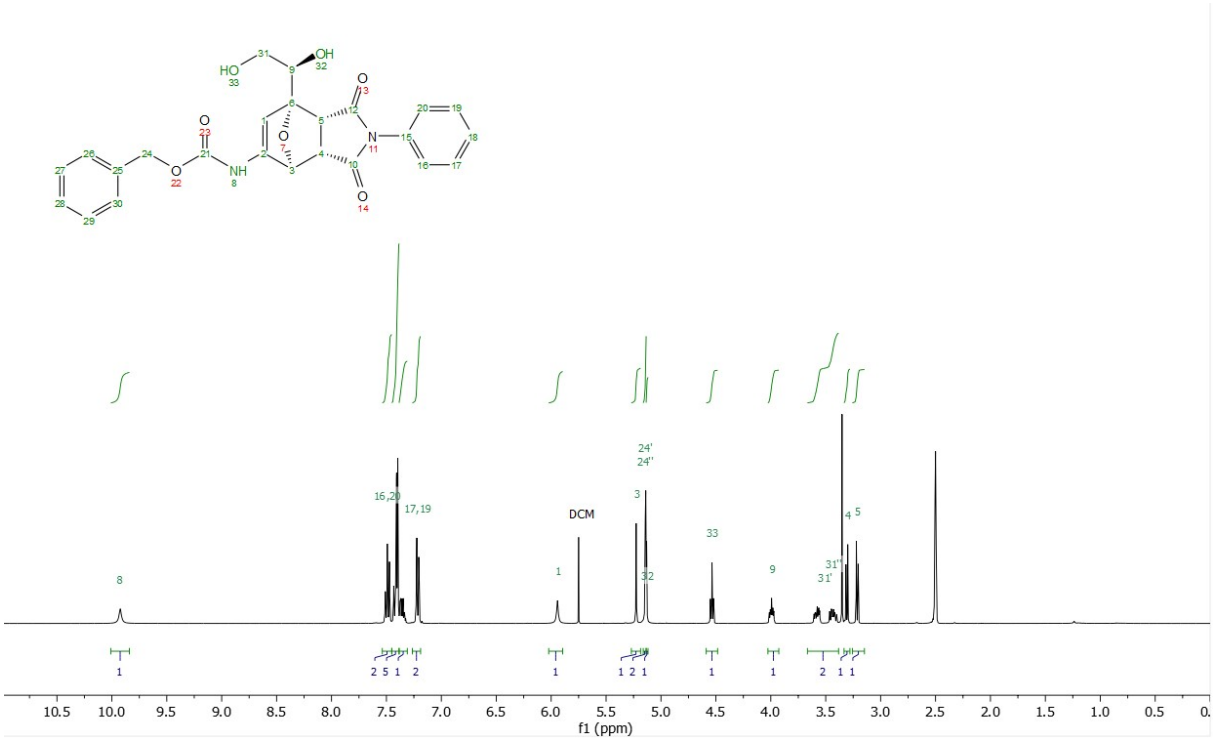


Processed Channel: PDA Ch1 210nm@4.8nm -Compens.

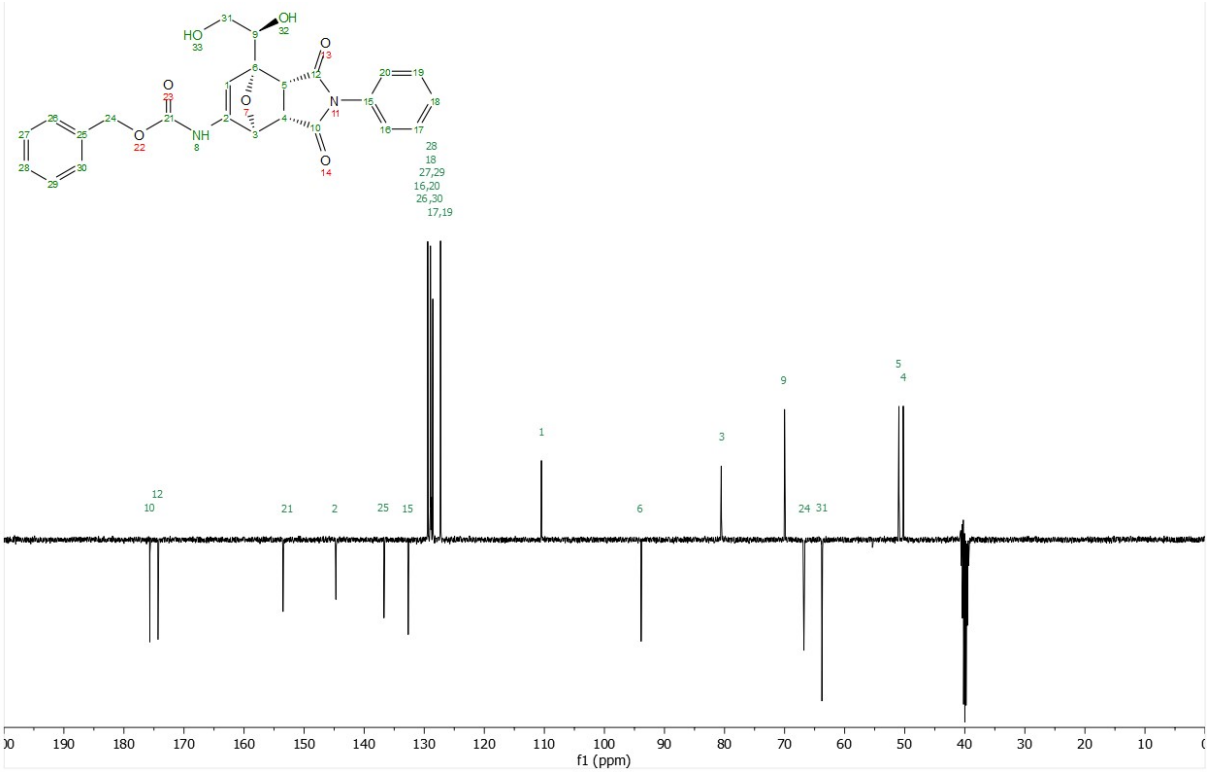
	RT (Min)	Area	Height	Area %
1	5.798	4162073	1121923	98.73
2	6.152	53498	15690	1.27

S14. DAP (**14**)

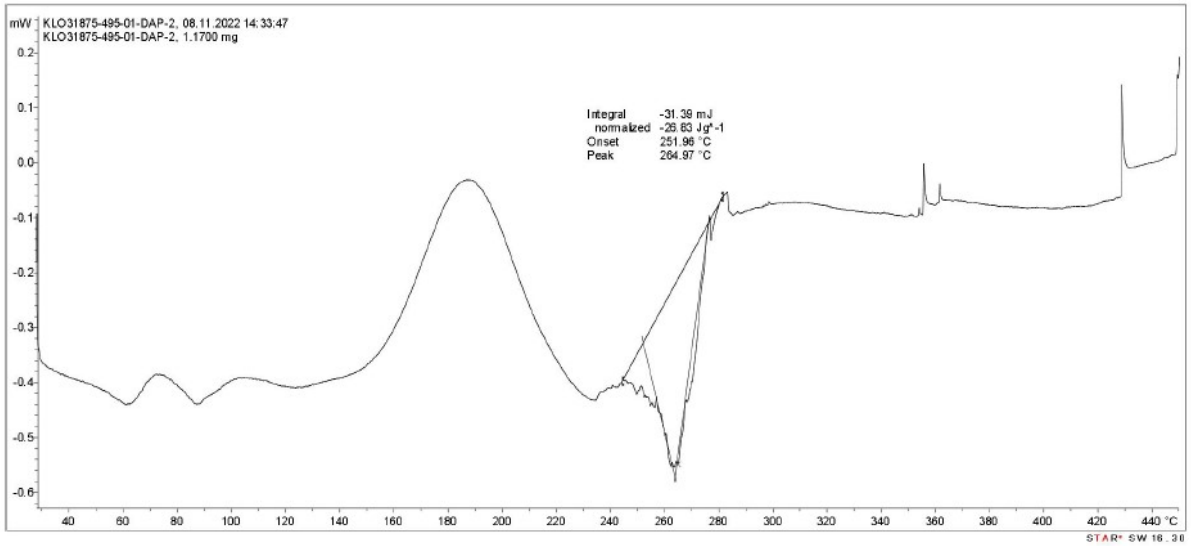
^{1}H-NMR of DAP (**14**) in DMSO-d_6



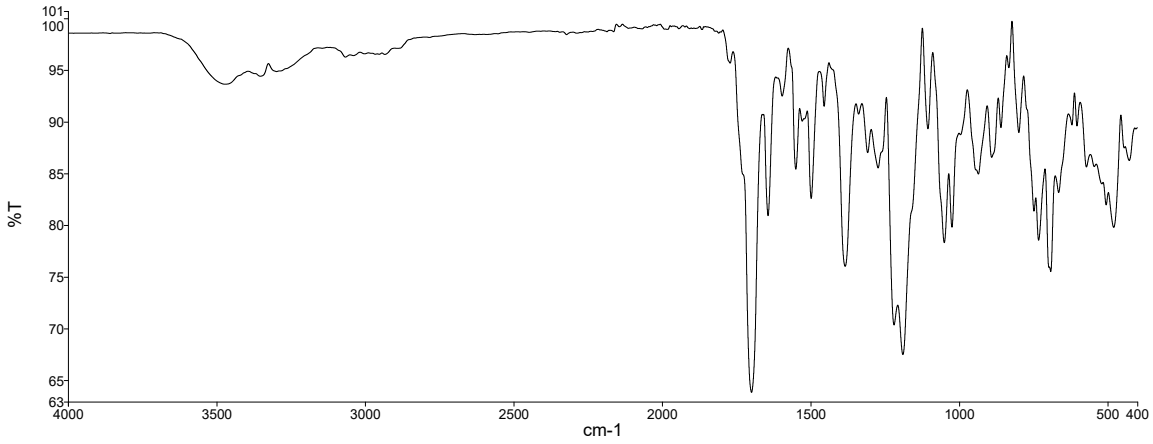
^{13}C-NMR of DAP (**14**) in DMSO-d_6



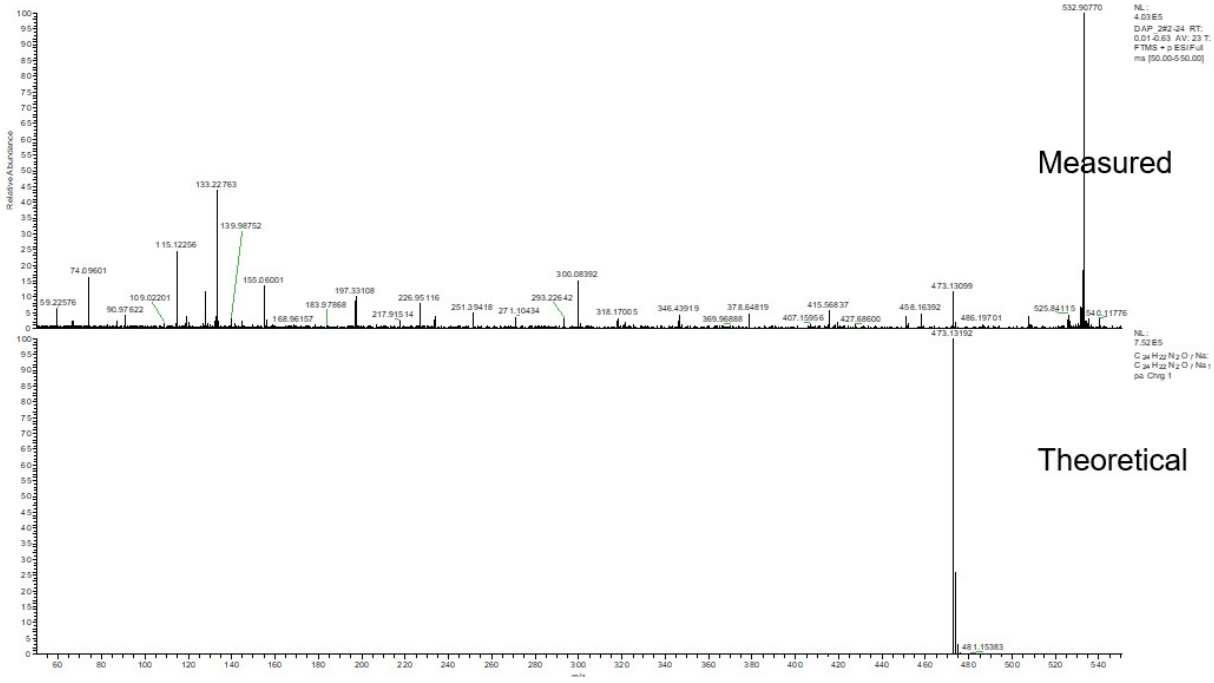
DSC of DAP (**14**)

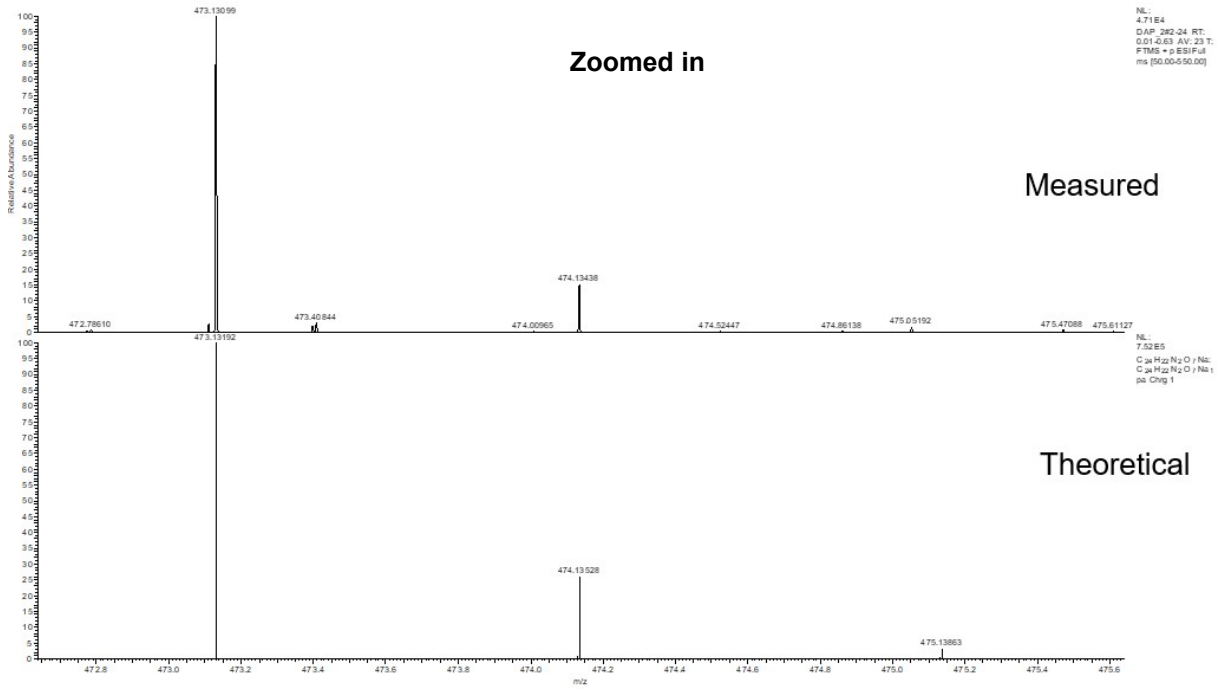


IR of DAP (**14**)



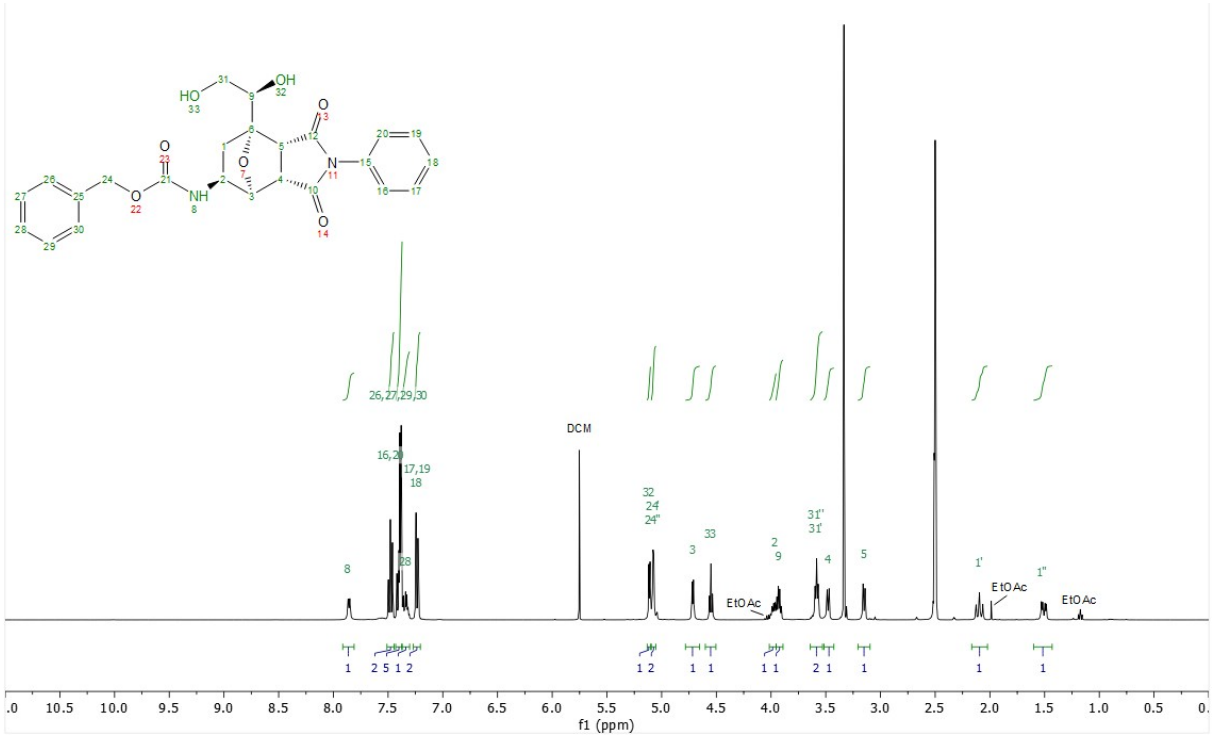
HRMS of DAP (**14**)



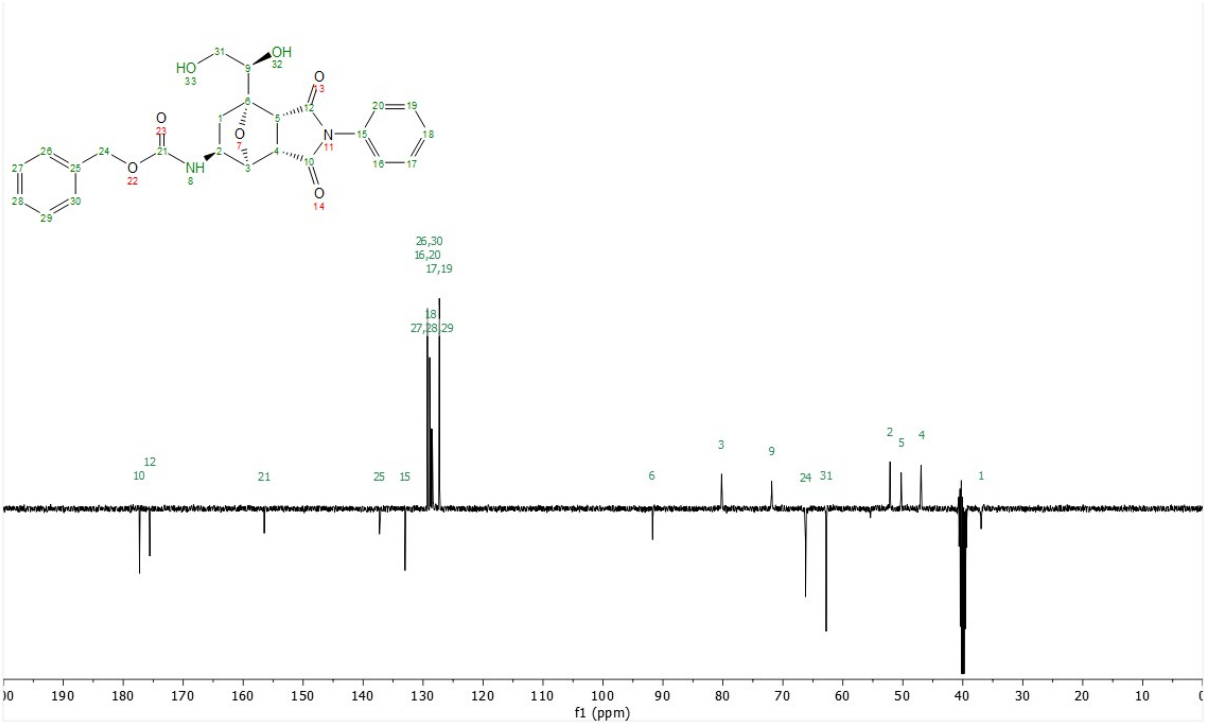


S15. DAPRED (**15**)

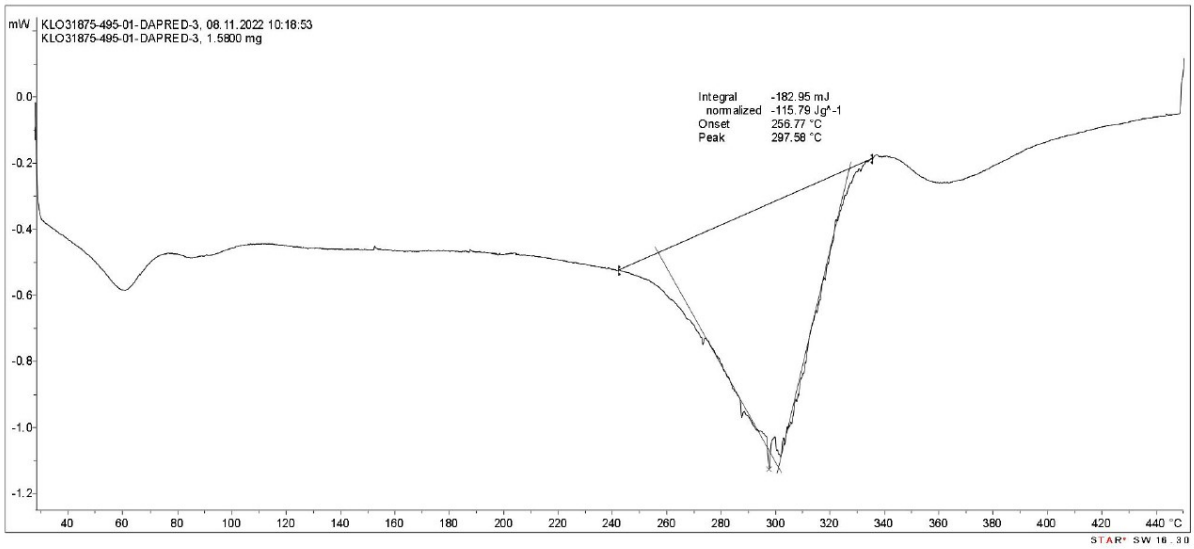
^{1}H-NMR of DAPRED (**15**) in DMSO-d_6



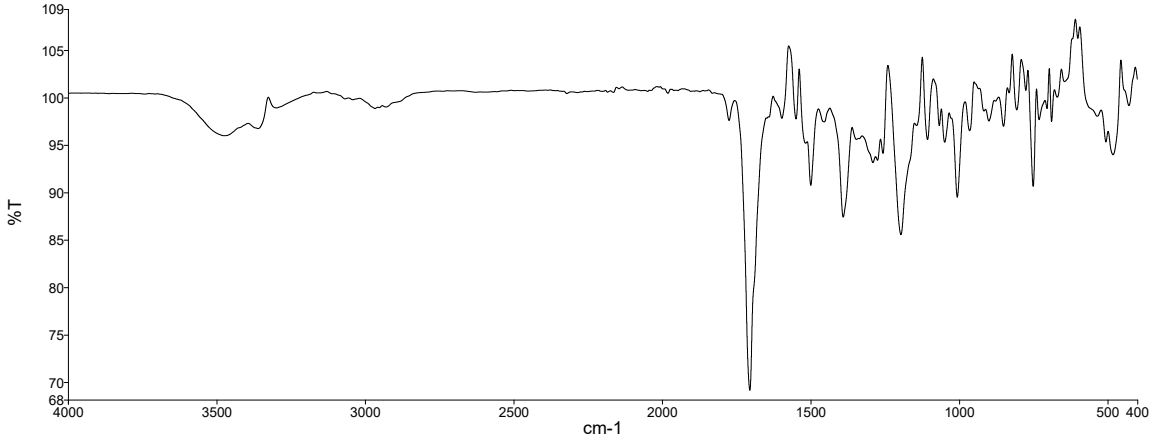
^{13}C-NMR of DAPRED (**15**) in DMSO-d_6



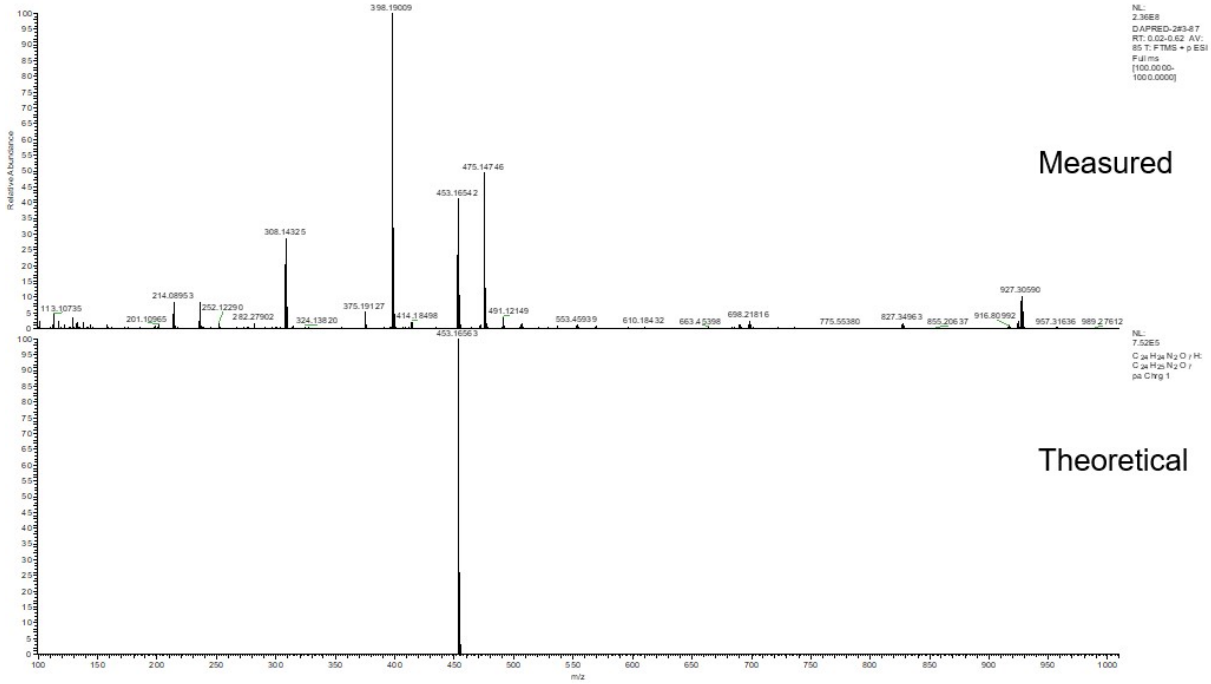
DSC of DAPRED (**15**)

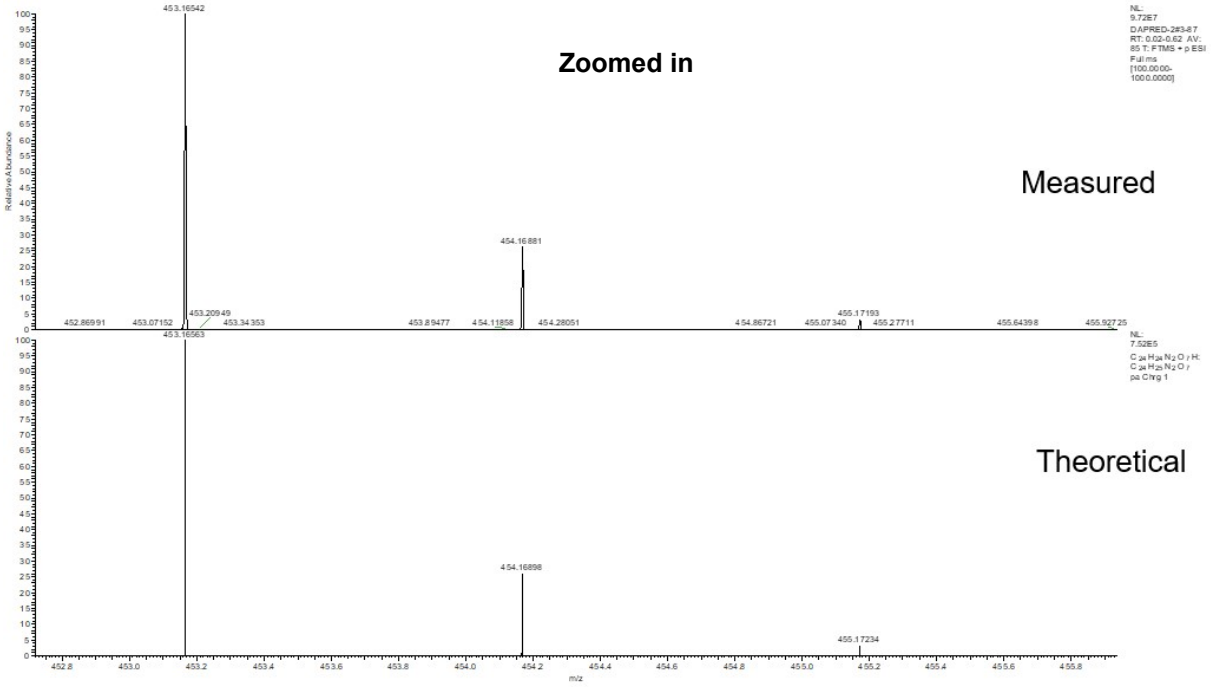


IR of DAPRED (**15**)



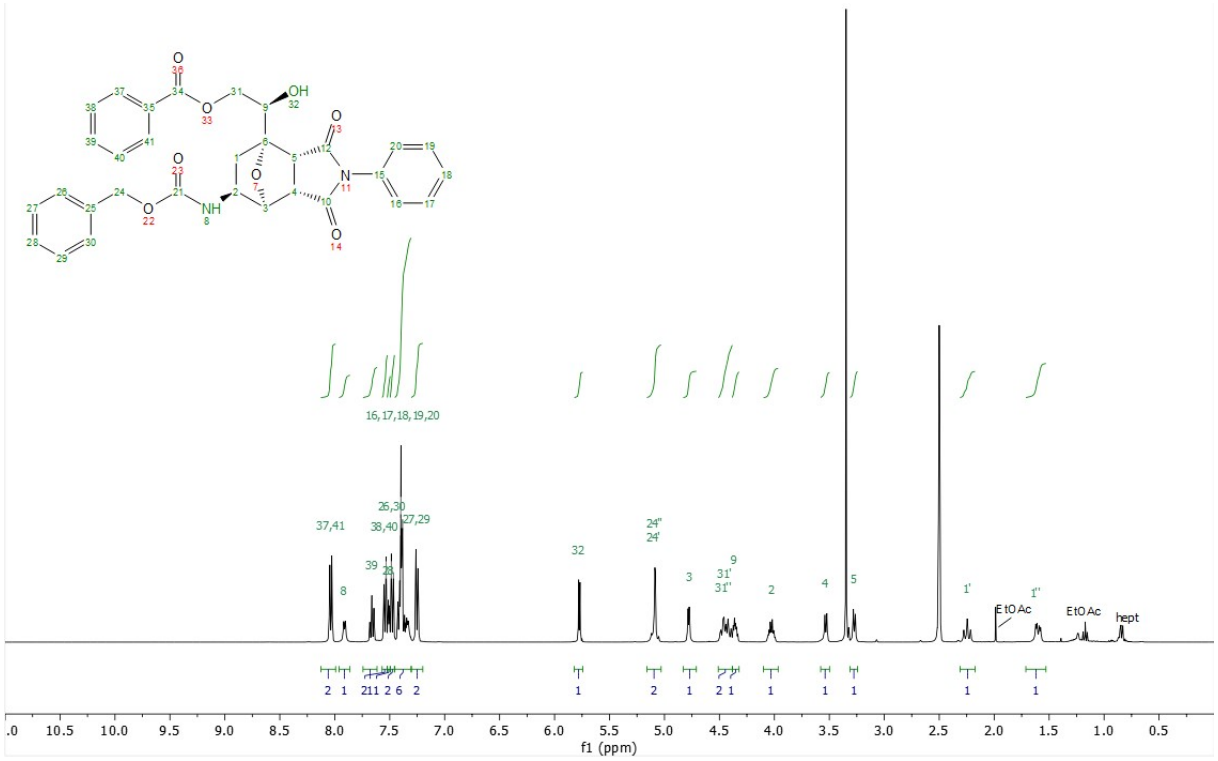
HRMS of DAPRED (**15**)



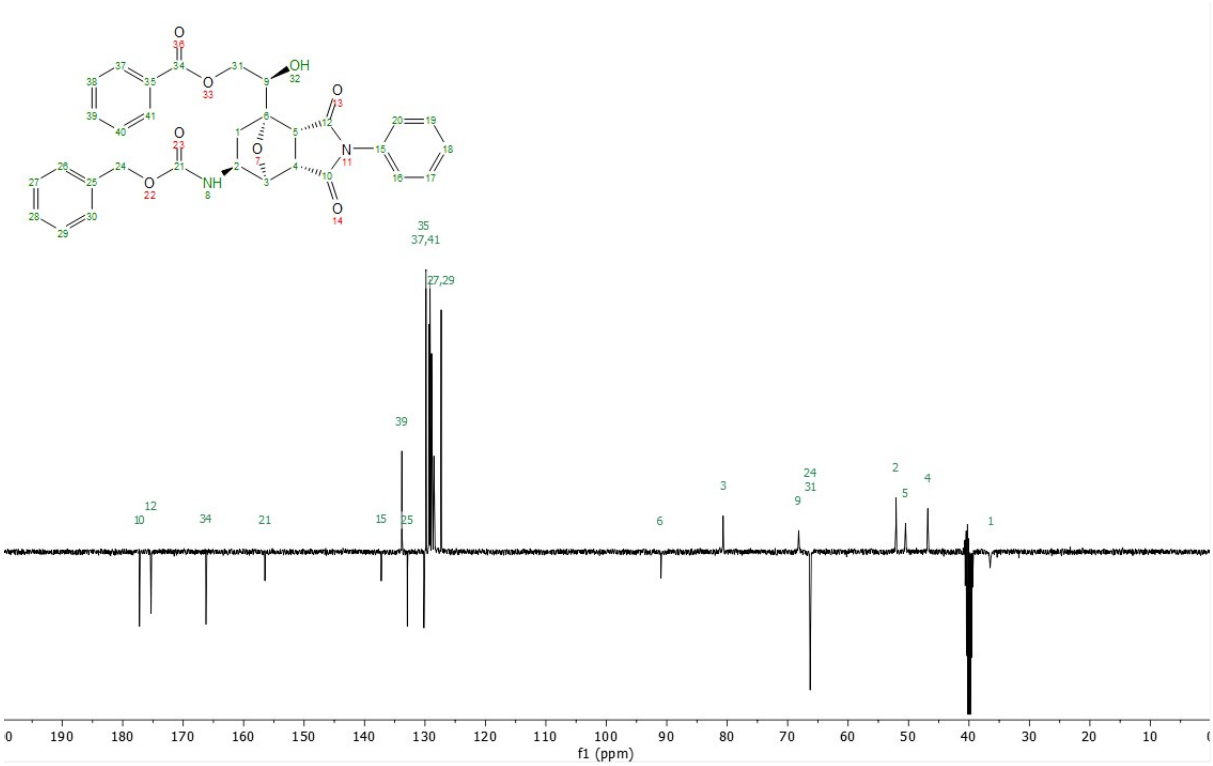


S16. DAPRED-Bz (**16**)

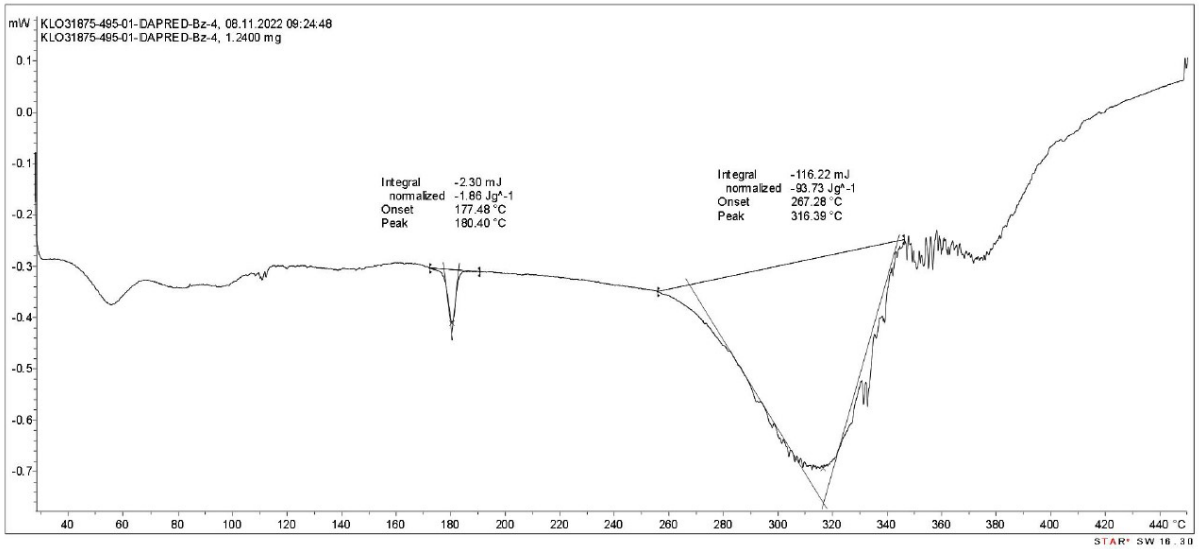
^{1}H-NMR of DAPRED-Bz (**16**) in DMSO-d_6



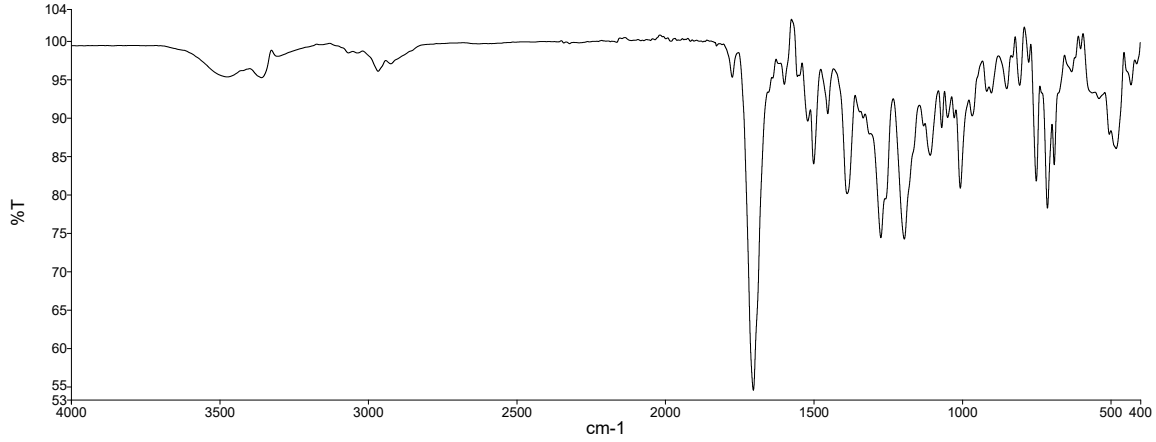
^{13}C-NMR of DAPRED (**16**) in DMSO-d_6



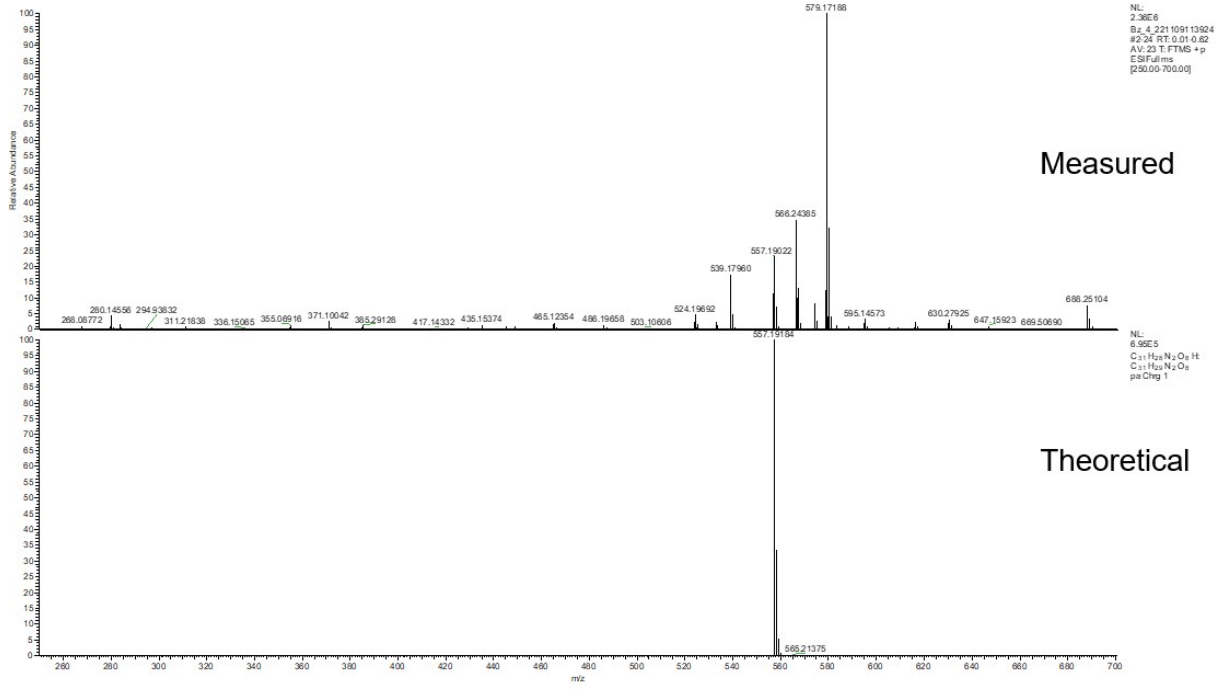
DSC of DAPRED-Bz (**16**)

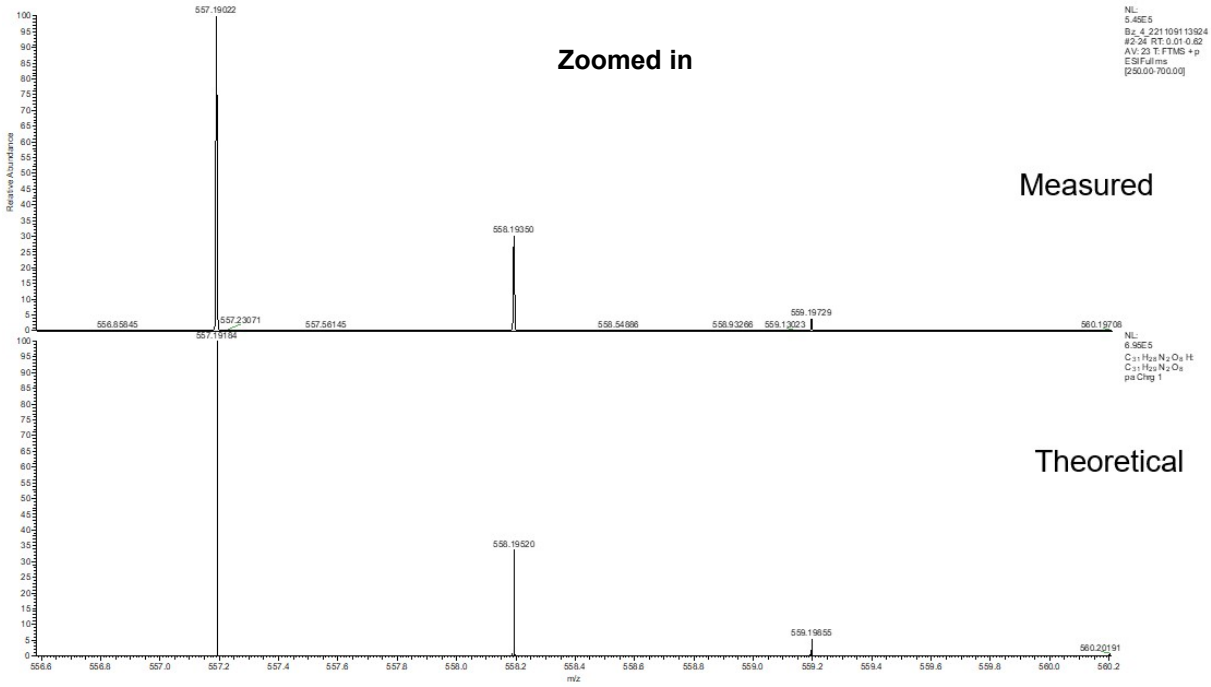


IR of DAPRED-Bz (**16**)



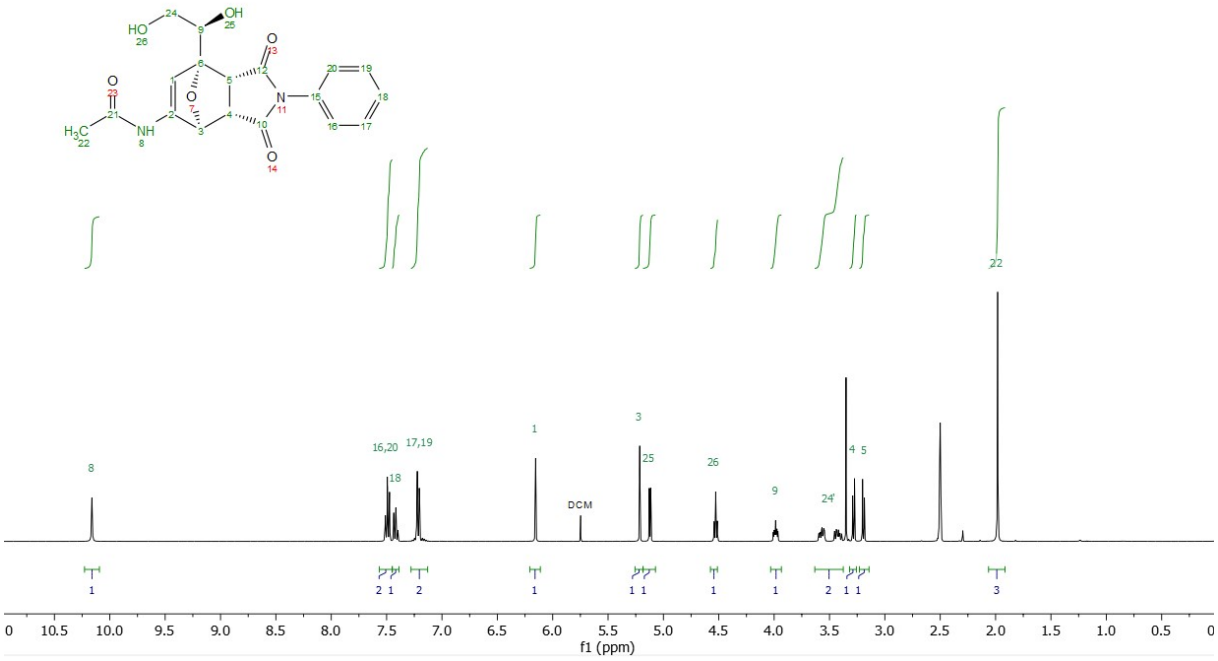
HRMS of DAPRED-Bz (**16**)



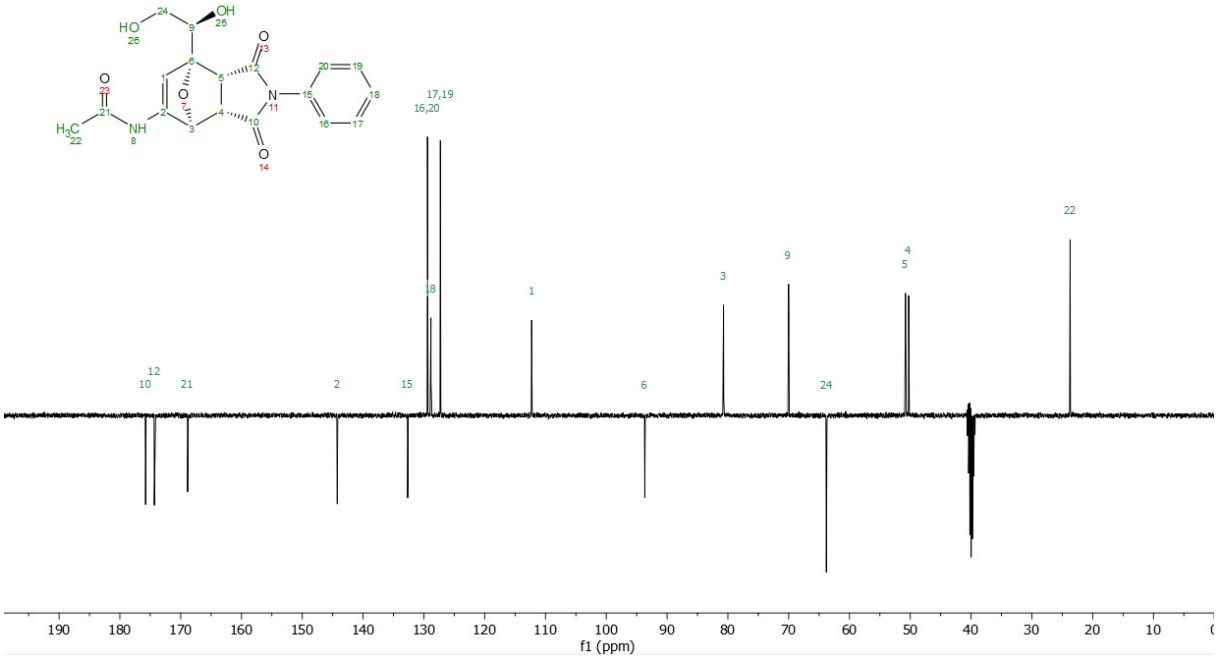


S17. Compound **18**

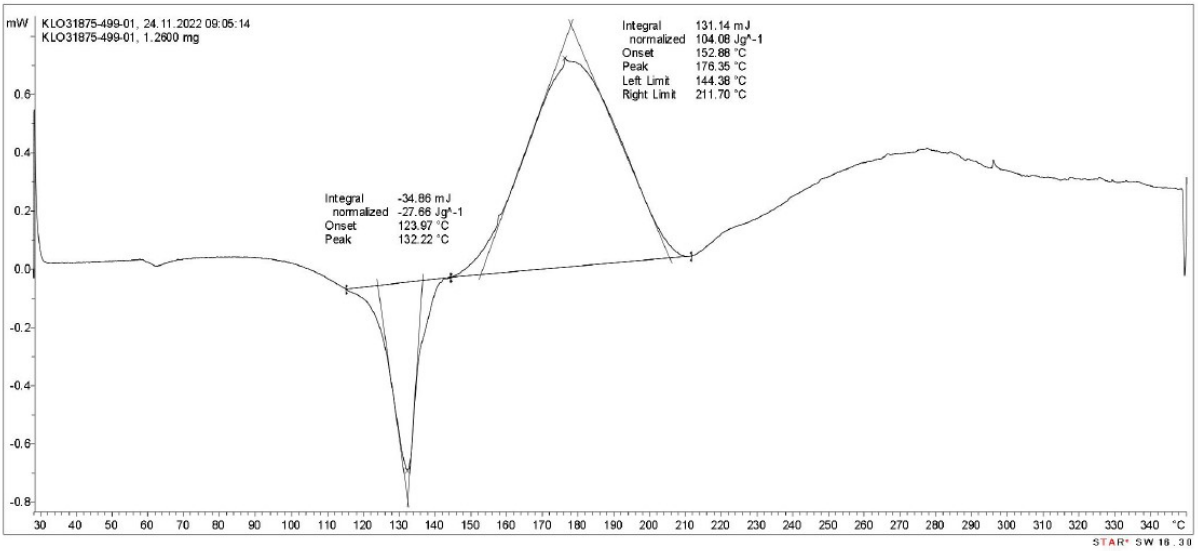
^{1}H-NMR of **18** in DMSO-d_6



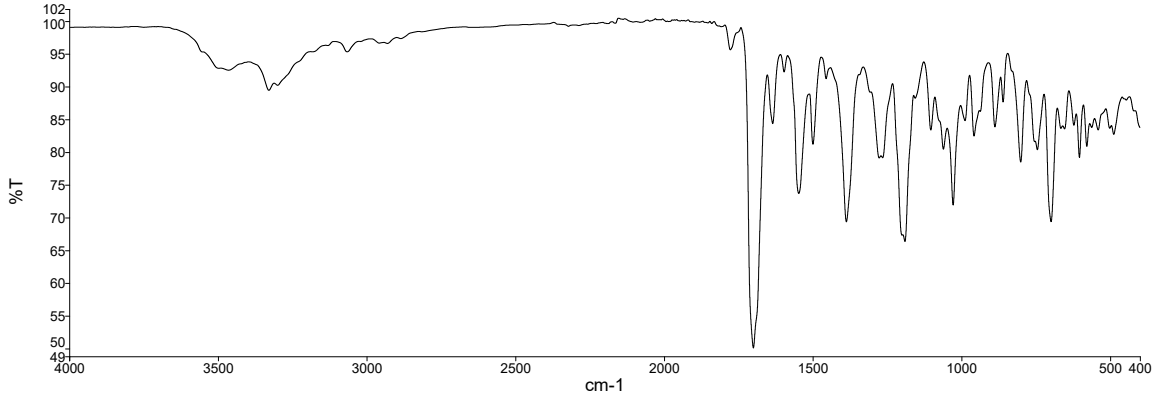
^{13}C-NMR of **18** in DMSO-d_6



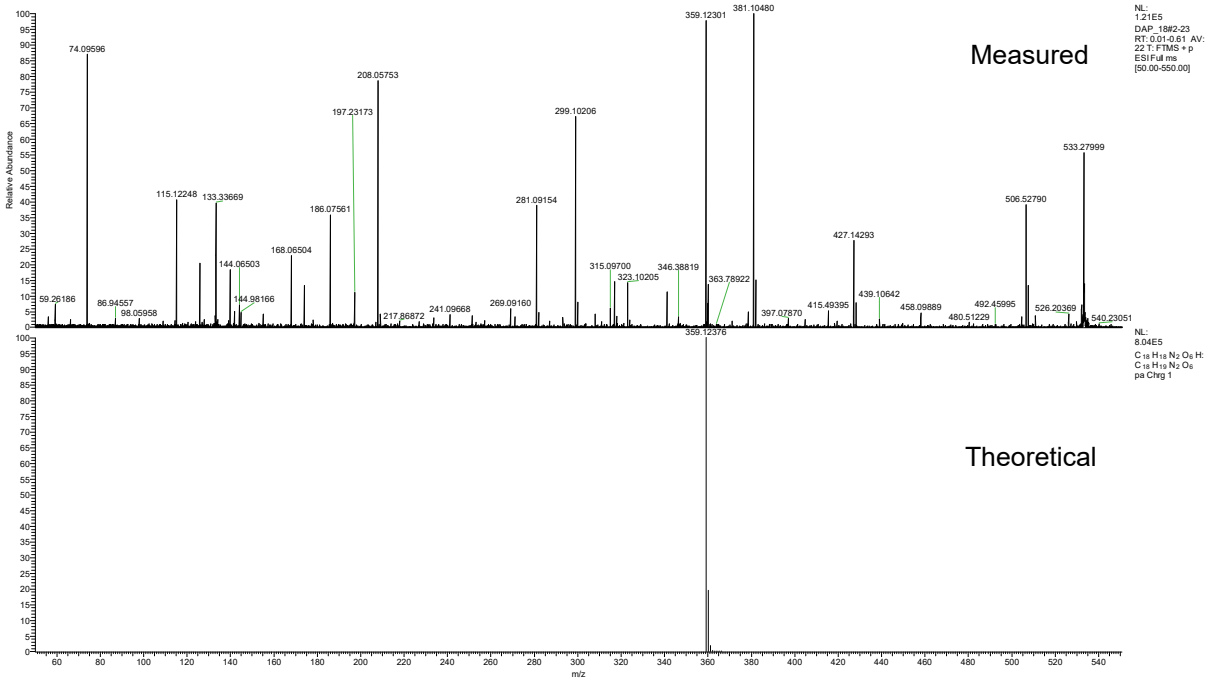
DSC of **18**

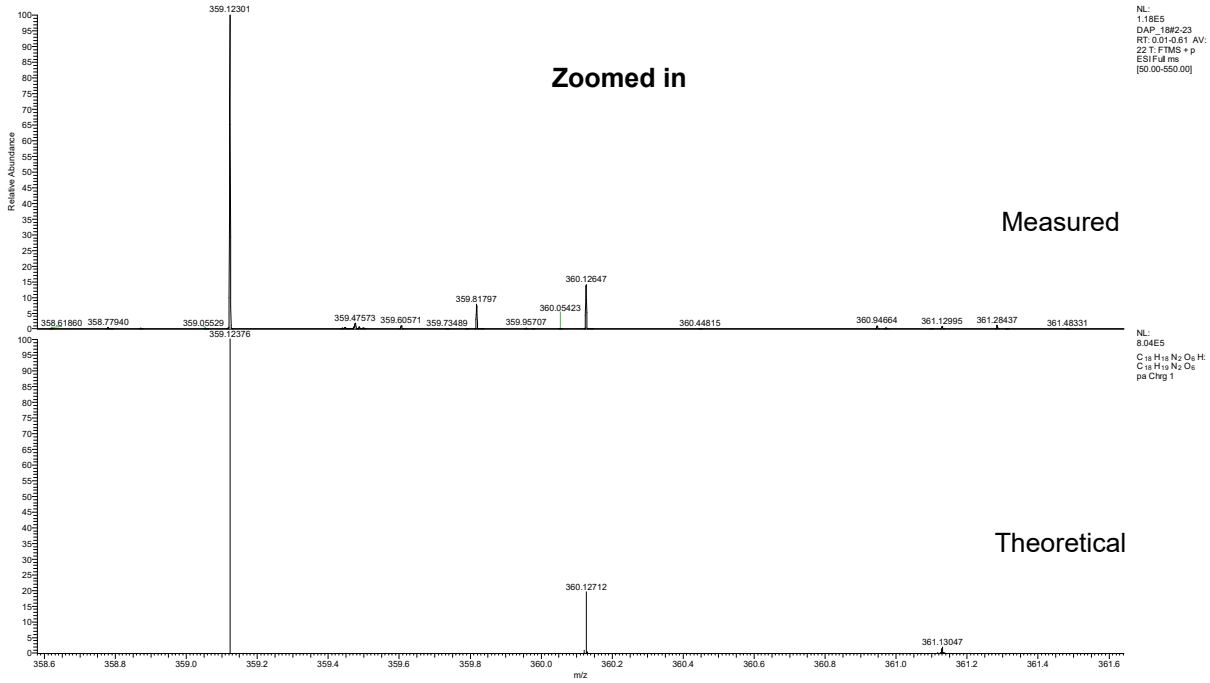


IR of **18**



HRMS of **18**




Zoomed in
Measured
Theoretical
Relative Abundance
m/z
NL:
1.18E5
DAP_18#2-23
RT: 0.01-0.61 AV:
22 T: FTMS + p
ESI Full ms
[50.00-550.00]
NL:
8.04E5
C18 H18 N2 O6 H:
C18 H19 N2 O6
pa Chrg 1
359.12301
360.12647
359.81797
360.05423
358.61860
358.77940
359.05529
359.47573
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